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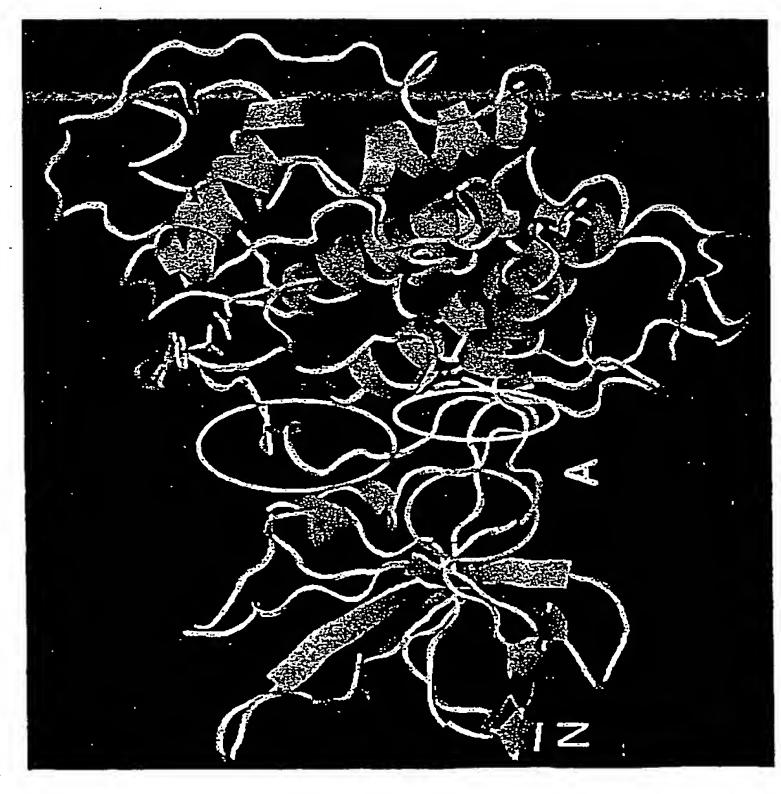
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(54) Title: CHARACTERIZATION OF THE GSK-3β PROTEIN AND METHODS OF USE THEREOF



(57) Abstract: The invention provides the three-dimensional structure of a construct of human glycogen synthase kinase 3 (GSK3); crystals of a construct of human glycogen synthase kinase 3-β (GSK3-β); containing the protein's catalytic kinase domain; a domain for crystallizing the protein construct to provide a GSK3 crystal sufficient for structure determination; and a method for using the GSK3 construct's three dimensional structure for the identification of possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3 activity.

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CHARACTERIZATION OF THE GSK-3 β PROTEIN AND METHODS OF USE THEREOF

FIELD OF THE INVENTION.

This invention relates to the three-dimensional structure of human glycogen synthase kinase 3 (GSK3), to crystals of a construct of GSK3, to methods for forming crystals of the GSK3 construct, to methods for determining the crystal structure of the GSK3 construct, and to methods for using the three-dimensional structure of GSK3 to identify possible therapeutic compounds for the treatment of various disease conditions mediated by GSK3 activity.

BACKGROUND OF THE INVENTION

Glycogen synthase kinase 3 (GSK3) is a serine/threonine kinase for which two isoforms, α and β , have been identified. Woodgett, *Trends Biochem. Sci.*, 16:177-81 (1991). Both GSK3 isoforms are constitutively active in resting cells. GSK3 was originally identified as a kinase that inhibits glycogen synthase by direct phosphorylation. Upon insulin activation, GSK3 is inactivated, thereby allowing the activation of glycogen synthase and possibly other insulin-dependent events, such as glucose transport. Subsequently, it has been shown that GSK3 activity is also inactivated by other growth factors that, like insulin, signal through receptor tyrosine kinases (RTKs). Examples of such signaling molecules include IGF-1 and EGF.

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Saito et al., Biochem. J., 303:27-31 (1994); Welsh et al., Biochem. J. 294:625-29 (1993); and Cross et al., Biochem. J., 303:21-26 (1994).

Agents that inhibit GSK3 activity are useful in the treatment of disorders that are mediated by GSK3 activity. In addition, inhibition of GSK3 mimics the activation of growth factor signaling pathways and consequently GSK3 inhibitors are useful in the treatment of diseases in which such pathways are insufficiently active. Examples of diseases that can be treated with GSK3 inhibitors include diabetes, Alzheimer's disease, CNS disorders such as bipolar disorder, and immune potentiation-related conditions, among others.

Because inhibitors of GSK3 are useful in the treatment of many diseases, the identification of new inhibitors of GSK3 would be highly desirable. The present invention provides a method for identifying possible therapeutic compounds for the treatment of various disease conditions mediated by GSK3 activity. The method of the present invention utilizes the three-dimensional structure of a GSK3 construct that contains the protein's catalytic domain to identify possible therapeutic compounds and to optimize the structure of lead therapeutic compounds.

SUMMARY OF THE INVENTION

In accordance with the present invention, the three-dimensional structure of a construct of human glycogen synthase kinase 3 (GSK3) is provided.

In one aspect, the invention provides crystals of a construct of human glycogen synthase kinase 3- β (GSK3- β) containing the protein's catalytic kinase domain.

In another aspect of the invention, a method for crystallizing the protein construct to provide a GSK3 crystal sufficient for structure determination is provided.

In a further aspect, the three-dimensional structure of the GSK3 construct is provided.

In yet another aspect, a method is provided for using the GSK3 construct's three-dimensional structure for the identification of possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3 activity.

BRIEF DESCRIPTION OF THE DRAWINGS

The foregoing aspects and many of the attendant advantages of this invention will become more readily appreciated by reference to the following detailed description, when taken in conjunction with the accompanying drawings, wherein:

FIGURE 1 is an illustration of the structure of the GSK3- β construct;

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FIGURE 2 is an illustration of the structure of the GSK3-β construct active site;

FIGURE 3 is a flow diagram of a representative method of the invention using the three-dimensional structure of the GSK3-β.construct for identifying possible therapeutic compounds for mediating GSK3-β activity; and

FIGURE 4 is a flow diagram of a representative method of the invention using the three-dimensional structure of the GSK3-β construct for identifying possible therapeutic compounds for mediating GSK3-β activity.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENT

In accordance with the present invention, crystals of a protein construct of human glycogen synthase kinase 3- β (GSK3- β) containing the protein's catalytic kinase domain, methods for crystallizing the protein construct, the three-dimensional structure of the protein construct, and methods for using the three-dimensional structure for the identification of possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3- β activity are provided.

The GSK3-β Protein Construct: Expression, Purification, and Crystallization

In one aspect, the invention provides a composition that includes a GSK3-β construct that contains the protein's catalytic kinase domain. The construct includes at least residues 37-384 of human GSK3-β and lacks the 36 amino acids at the protein's C-terminus. The composition is a crystalline form sufficient for structure determination by diffraction studies by X-ray.

It will be appreciated that GSK3 protein constructs other than the construct described herein, for example, active mutants or variants thereof, can provide three-dimensional structural information useful in identifying possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3 activity.

Construct Sequence. The construct sequence, SEQ ID NO: 1, is provided below. The asterisk indicates the first residue that is seen in the crystal structure. The following construct and additional useful constructs and their preparation are described in co-pending U.S. Patent Application Serial No. 60/221,242, filed July 27, 2000, the disclosure of which is incorporated herein by reference in its entirety and for all purposes.

N-terminus: MEYMPMEGGGSK

*VTTVVATPGQGPDRPQEVSYTDTKVIGNGSFGVVYQAKLCDSGELV AIKKVLQDKRFKNRELQIMRKLDHCNIVRLRYFFYSSGEKKDEVYLNLVLDY

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VPETVYRVARHYSRAKQTLPVIYVKLYMYQLFRSLAYIHSFGICHRDIKPQN LLLDPDTAVLKLCDFGSAKQLVRGEPNVSYICSRYYRAPELIFGATDYTSSID VWSAGCVLAELLLGQPIFPGDSGVDQLVEIIKVLGTPTREQIREMNPNYTEFK FPQIKAHPWTKVFRPRTPPEAIALCSRLLEYTPTARLTPLEACAHSFFDELRDP NVKLPNGRDTPALFNFTTQELSSNPPLATILIPPHARI: C-terminus (SEQ ID NO: 1)

Construct Purification. The GSK3-β protein construct was extracted from SF-9 cells infected with a baculovirus carrying GSK3-β 580 cDNA construct. The GSK3-β protein construct was purified to apparent homogeneity using S-Fractogel, Phenyl-650 M, and Glu-tag affinity chromatographies. The purified protein was then concentrated for crystallization. Purification of the construct is described in Example 1.

Construct Crystallization. Protein crystals can be formed from solutions of the GSK3 construct by, for example, the hanging drop technique. A representative method for forming suitable crystals of the GSK3 construct suitable for structure determination is described in Example 2.

It will be appreciated that various crystallization methods including, for example, microcrystallization methods can be utilized to obtain three-dimensional structural information useful in identifying possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3 activity.

The GSK3-β Protein Construct Structure

In another aspect of the invention, the three-dimensional structure of the GSK3 protein construct is provided. Amino acid sequence data and atomic coordinates derived from X-ray diffraction data were used to determine the construct's three-dimensional structure. The construct's atomic coordinates were calculated from an electron density map produced from the combination of X-ray diffraction and phase data.

With the GSK3 construct available in crystalline form suitable for structural determination, the crystal structure can be obtained by a variety of techniques. In a representative method, diffraction patterns were obtained using an X-ray image plate device. Phase data was then obtained by a combination of molecular replacement and cross-crystal averaging techniques. Electron density maps were then constructed and the structure solved and molecule built. The resulting structure was refined and the structure validated. The ultimate result was an atomic model of the GSK3 construct. A representative method for obtaining the GSK3 crystal structure is described in Example 3.

It will be appreciated that the GSK3 structure can be solved by a variety of methods.

The statistics for collecting the crystallographic data are summarized in Table 1.

Table 1. Data and Model Statistics for Structure Solution.

	Native 2.2Å
Space Group	P222(1)
Highest Resolution (Å)	2.2
R _{merge} (%)	10.4
I/σ (total)	13.7
Final Shell	2.26Å – 2.20Å
I/Iσ (Final Shell)	3.3
R-factor (%)	26.2
free-R factor (%)	30.8

The three-dimensional structure of the GSK3-β construct provided as a tabulation of atomic coordinates is given in Table 2. In the table, "OH2" and "GOL" refer to structural water and glycerol molecules, and "TER" refers to the terminus of a peptide chain.

Table 2. GSK3-β Construct Atomic Coordinates.

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	ATOM	1	CB.	VAL A	37	80.033	24.831 -19.608	1.00 50.57
15	ATOM	2	CG1	VAL A	37	81.501	25.233 -19.582	1.00 50.37
	ATOM	3	CG2	VAL A	37	79.466	24.947 -21.017	1.00 51.61
	ATOM	4	С	VAL A	37	80.398	23.336 -17.638	1.00 50.20
	ATOM	5	0	VAL A	37	79.972	24.095 -16.767	1.00 51.05
	ATOM	6	N	VAL A	37	78.411	22.987 -19.067	1.00 49.79
20	ATOM .	7	CA	VAL A	37	79.846	23.399 -19.056	1.00 50.62
	ATOM	8	N	THR A	38	81.331	22.418 -17.401	1.00 49.02
	MOTA	9	CA	THR A	38	81.900	22.262 -16.068	1.00 48.04
	ATOM	10	СВ	THR A	38	81.970	20.789 -15.652	1.00 48.38
	ATOM	11	OG1	THR A	38	83.312	20.328 -15.604	1.00 49.77
25	ATOM	12	CG2	THR A	38	81.167	19.848 -16.525	1.00 47.77
	ATOM	13	С	THR A	38	83.262	22.918 -15.914	1.00 47.01

	7 most	3.4	_	6					_	_
	ATOM	14	0	THR A		84.143		-16.755		
	ATOM	15	N	THR A		83.436	23.626 -		1.00	45.08
	MOTA	16	CA	THR A	39	84.701	24.275 -	-14.508	1.00	42.86
_	MOTA	17	CB	THR A	39	84.538	25.790 -	-14.267	1.00	43.86
5	ATOM	18	OG1	THR A	39	84.623	26.130 -	-12.895	1.00	44.44
	ATOM	19	CG2	THR A	39	83.258	26.382 -	-14.821	1.00	43.65
	MOTA	20	С	THR A	39	85.395	23.571 -	-13.338	1.00	40.74
	MOTA	21	0	THR A	39	84.759	23.220 -	-12.334	1.00	40.93
	ATOM	22	N	VAL A	40	86.694	23.349 -	-13.485	1.00	38.40
10	ATOM	23	CA	VAL A	40	87.483	22.679 -	-12.464	1.00	35.30
	ATOM	24	CB	VAL A	40	88.180	21.427 -	-13.027	1.00	34.48
	ATOM	25	CG1	VAL A	40	89.077	20.788 -	-11.983	1.00	34.49
	ATOM	26	CG2	VAL A	40	87.142	20.429 -	-13.516	1.00	34.61
	ATOM	27	C	VAL A	40	88.513	23.636 -	-11.873	1.00	34.74
15	ATOM	28	0	VAL A	40	89.329	24.220 -	-12.601	1.00	33.31
	ATOM	29	N	VAL A	41	88.454	23.806 -	-10.543	1.00	33.24
•	MOTA	30	CA	VAL A	41 .	89.362	24.707	-9.838	1.00	30.39
	ATOM	31	CB	VAL A	41	88.589	25.899	-9.223	1.00	31,41
	ATOM	32	CG1	VAL A	41	87.840	26.681 -	-10.294	1.00	28.06
20	MOTA	33	CG2	VAL .A	41	87.632	25.422	-8.136	1.00	29.89
	ATOM	34	С	VAL A	41	90.122	23.990	-8.723	1.00	29.47
	ATOM	35	0	VAL A	41 .	89.751	22.891	-8.311	1.00	28.80
	MOTA	36	N	ALA A	42	91.167	24.638	-8.219	1.00	28.13
	ATOM	37	CA	ALA A	42	91.960	24.092	-7.119	1.00	29.60
25	ATOM	38	CB	ALA A	42	93.450	24.229	-7.400	1.00	28.11
	MOTA	39	С	ALA A	42	91.581	24.837	-5.835	1.00	29.66
	MOTA	40	0	ALA A	42	91.963	25, 990	-5.648	1.00	28.27
	MOTA	41	N	THR A	43	90.789	24.196	-4.981	1.00	30.99
	MOTA	42	CA	THR A	43	90.337	24.849	-3.762	1.00	34.40
30	MOTA	43	СВ	THR A	43	88.911	25.332	-3.955	1.00	36.00
	MOTA	44	OG1	THR A	43	88.371	25.782	-2.727	1.00	43.97
	MOTA	45	CG2	THR A	43	87.985	24.275	-4.510	1.00	37.41
	ATOM	46	С	THR A	43	90.408	23.974	-2.506	1.00	33.11
	ATOM	47	0	THR A	43	90.083	22.791	-2.538	1.00	33.54
35	ATOM	48	N	PRO A	44	90.826	24.572	-1.375	1.00	32.56

ATOM	49	CD	PRO	A	44	91.239	25.963 -	1.245	1.00	35.07
ATOM	50	CA	PRO	A	44	90.930	23.899 -	-0.087	1.00	33.94
MOTA	51	CB	PRO	A	44	92.056	24.682	0.621	1.00	33.35
ATOM	52	CG	PRO	A	44	92.363	25.860	-0.251	1.00	33.23
ATOM	53	С	PRO	A	44	89.646	24.069	Ò.709	1.00	32.73
MOTA	54	0	PRO	A	44	88.967	25.089	0.591	1.00	31.50
MOTA	55	N	GLY	A	45	89.324	23.087	1.532	1.00	35.79
ATOM	56	CA	GLY	A	45	88.123	23.201	2.342	1.00	39.32
ATOM	57 .	C	GLY	A	45 .	88.377	24.052	3.576	1.00	41.20
MOTA	58	0	GLY	A	45	89.460	24.624	3.724	1.00	38.49
ATOM	59	N	GLN	A	46	87.399	24.114	4.483	1.00	46.21
MOTA	60	CA.	GLN	A	46	87.570	24.868	5.729	1.00	48.58
MOTA	61	CB	GLN	A	46	86.280	25.586	6.143	1.00	50.56
MOTA	62	CG	GLN	A	46	85.157	24.661	6.612	1.00	53.97
MOTA	63	CD	GLN	A	46	84.699	24.926	8.044	1.00	54.45
ATOM	64	OE1	GLN	A	46	85.143	25.874	8.699	1.00	54.99
ATOM	65	NE2	GLN	À	46	83.801	24.083	8.535	1.00	54.65
ATOM	66	C	GLN	A	46	88.035	23.908	6.822	1.00	49.85
MOTA	67	0	GLN	A	46	87.531	23.929	7.948	1.00	50.43
MOTA	68	N	GLY	A	47	88.992	23.042	6.465	1.00	50.37
ATOM	69	CA	GLY	A	47	89.492	22.066	7.410	1.00	51.27
ATOM	70	С	GLY	A	47	91.005	21.903	7.413	1.00	51.26
ATOM	71	0	GLY	A	47	91.731	22.809	7.831	1.00	51.04
ATOM	72	N	PRO	A	48	91.504	20.724	6.987	1.00	51.25
ATOM	73	CD	PRO	A	48	90.694	19.579	6.520	1.00	52.23
ATOM	74	CA	PRO	A	48	92.939	20.413	6.984	1.00	51.17
MOTA	75	CB	PRO	A	48	92.949	18.883	6.954	1.00	51.98
ATOM	76	CG	PRO	A	48	91.722	18.526	6.185	1.00	52.45
MOTA	77	С	PRO	A	48	93.703	20.964	5.785	1.00	50.33
ATOM	78	0	PRO	A	48	94.648	20.331	5.310	1.00	51.68
ATOM	79	N	ASP	A	49	93.312	22.141	5.305	1.00	48.80
MOTA	80	CA	ASP	A	49	93.991	22.755	4.165	1.00	48.33
'ATOM	81	CB	ASP	A	49	95.381	23.259	4.595	1.00	48.73
MOTA	82	CG	ASP	A	49	95.853	24.465	3.805	1.00	49.64
MOTA	83	OD1	ASP	A	49	96.434	24.267	2.722	1.00	51.08
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 51 ATOM 52 ATOM 53 ATOM 54 ATOM 55 ATOM 56 ATOM 57 ATOM 58 ATOM 60 ATOM 61 ATOM 62 ATOM 63 ATOM 63 ATOM 65 ATOM 65 ATOM 65 ATOM 65 ATOM 67 ATOM 68 ATOM 67 ATOM 70 ATOM 71 ATOM 72 ATOM 73 ATOM 74 ATOM 75 ATOM 75 ATOM 76 ATOM 77 ATOM 77 ATOM 78 ATOM 79	ATOM 50 CA ATOM 51 CB ATOM 52 CG ATOM 53 C ATOM 54 O ATOM 55 N ATOM 56 CA ATOM 57 C ATOM 59 N ATOM 61 CB ATOM 62 CG ATOM 63 CD ATOM 65 NE2 ATOM 66 C ATOM 67 O ATOM 69 CA ATOM 70 C ATOM 71 O ATOM 72 N ATOM 73 CD ATOM 74 CA ATOM 75 CB ATOM 76 CG ATOM 77 C ATOM 77 C ATOM 77 C ATOM 78 O ATO	ATOM 50 CA PRO ATOM 51 CB PRO ATOM 52 CG PRO ATOM 54 O PRO ATOM 55 N GLY ATOM 56 CA GLY ATOM 57 C GLY ATOM 59 N GLN ATOM 61 CB GLN ATOM 62 CG GLN ATOM 64 OE1 GLN ATOM 65 NE2 GLN ATOM 66 C GLN ATOM 67 O GLY ATOM 69 CA GLY ATOM 70 C GLY ATOM 71 O GLY ATOM 72 N PRO ATOM 74 CA PRO ATOM 75 CB PRO	ATOM 50 CA PRO A ATOM 51 CB PRO A ATOM 52 CG PRO A ATOM 54 O PRO A ATOM 55 N GLY A ATOM 56 CA GLY A ATOM 57 C GLY A ATOM 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23.899 - ATOM 51 CB PRO A 44 92.056 24.682 ATOM 52 CG PRO A 44 92.363 25.860 - ATOM 53 C PRO A 44 89.646 24.069 ATOM 54 O PRO A 44 88.967 25.089 ATOM 55 N GLY A 45 89.324 23.087 ATOM 56 CA GLY A 45 88.123 23.201 ATOM 57 C GLY A 45 88.377 24.052 ATOM 58 O GLY A 45 89.460 24.624 ATOM 59 N GLN A 46 87.399 24.114 ATOM 60 CA GLN A 46 87.399 24.114 ATOM 61 CB GLN A 46 86.280 25.586 ATOM 63 CD GLN A 46 85.157 24.661 ATOM 64 OE1 GLN A 46 85.157 24.661 ATOM 65 NE2 GLN A 46 83.801 24.083 ATOM 66 C GLN A 46 83.801 24.083 ATOM 66 C GLN A 46 83.801 24.083 ATOM 66 C GLN A 46 83.801 24.083 ATOM 67 O GLN A 46 83.801 24.083 ATOM 68 N GLY A 47 88.992 23.042 ATOM 69 CA GLY A 47 89.492 22.066 ATOM 70 C GLY A 47 89.492 22.066 ATOM 71 O GLY A 47 91.005 21.903 ATOM 72 N PRO A 48 91.504 20.724 ATOM 73 CD PRO A 48 92.939 20.413 ATOM 76 CG PRO A 48 92.939 20.413 ATOM 77 C PRO A 48 92.939 20.413 ATOM 76 CG PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 92.949 18.883 ATOM 76 CG PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 93.703 20.964 ATOM 78 O PRO A 48 93.703 20.964 ATOM 79 N ASP A 49 93.312 22.141 ATOM 79 N ASP A 49 93.991 22.755 ATOM 78 C PRO A 48 93.991 22.755 ATOM 78 C PRO A 49 93.991 22.755 ATOM 81 CB ASP A 49 95.381 23.259</td> <td>ATOM 50 CA PRO A 44 90.930 23.899 -0.087 ATOM 51 CB PRO A 44 92.056 24.682 0.621 ATOM 52 CG PRO A 44 92.363 25.860 -0.251 ATOM 53 C PRO A 44 89.646 24.069 0.709 ATOM 54 O PRO A 44 88.967 25.089 0.591 ATOM 55 N GLY A 45 89.324 23.087 1.532 ATOM 56 CA GLY A 45 88.123 23.201 2.342 ATOM 57 C GLY A 45 89.460 24.624 3.724 ATOM 59 N GLN A 46 87.399 24.114 4.483 ATOM 59 N GLN A 46 87.399 24.114 4.483 ATOM 60 CA GLN A 46 87.570 24.868 5.729 ATOM 61 CB GLN A 46 85.157 24.661 6.612 ATOM 63 CD GLN A 46 85.157 24.661 6.612 ATOM 64 OE1 GLN A 46 85.143 25.874 8.699 ATOM 65 NE2 GLN A 46 85.143 25.874 8.699 ATOM 65 NE2 GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 67 O GLN A 46 88.992 23.042 6.465 ATOM 68 N GLY A 47 88.992 23.042 6.465 ATOM 69 CA GLY A 47 88.992 23.042 6.465 ATOM 69 CA GLY A 47 89.492 22.066 7.410 ATOM 69 CA GLY A 47 89.492 22.066 7.410 ATOM 69 CA GLY A 47 91.005 21.903 7.413 ATOM 71 O GLY A 47 91.005 21.903 7.413 ATOM 72 N PRO A 48 91.504 20.724 6.987 ATOM 73 CD PRO A 48 92.939 20.413 6.984 ATOM 74 CA PRO A 48 92.939 20.413 6.984 ATOM 75 CB PRO A 48 92.939 20.413 6.984 ATOM 76 CG PRO A 48 92.939 20.413 6.984 ATOM 76 CG PRO A 48 92.939 20.413 6.984 ATOM 76 CG PRO A 48 92.939 20.413 6.984 ATOM 77 C PRO A 48 92.939 20.413 6.984 ATOM 77 C PRO A 48 92.939 20.413 6.984 ATOM 77 C PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 ATOM 78 O PRO A 48 92.939 20.413 6.984 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64 OE1 GLN A 46 ATOM 66 C GLN A 46 ATOM 66 C GLN A 46 ATOM 67 O GLN A 46 ATOM 68 N GLY A 47 ATOM 69 CA GLY A 47 ATOM 70 C GLY A 47 ATOM 70 C GLY A 47 ATOM 71 O GLY A 47 ATOM 72 N PRO A 48 ATOM 73 CD PRO A 48 ATOM 74 CA PRO A 48 ATOM 76 CG PRO A 48 ATOM 76 CG PRO A 48 ATOM 76 CG PRO A 48 ATOM 77 C PRO A 48 ATOM 78 O PRO A 48 ATOM 79 N ASP A 49	ATOM 50 CA PRO A 44 90.930 ATOM 51 CB PRO A 44 92.056 ATOM 52 CG PRO A 44 92.363 ATOM 53 C PRO A 44 89.646 ATOM 54 O PRO A 44 88.967 ATOM 55 N GLY A 45 89.324 ATOM 56 CA GLY A 45 88.123 ATOM 57 C GLY A 45 89.460 ATOM 59 N GLY A 45 89.460 ATOM 59 N GLN A 46 87.399 ATOM 60 CA GLN A 46 87.570 ATOM 61 CB GLN A 46 85.157 ATOM 62 CG GLN A 46 85.157 ATOM 63 CD GLN A 46 85.157 ATOM 65 NE2 GLN A 46 83.801 ATOM 66 C GLN A 46 83.801 ATOM 67 O GLN A 46 87.531 ATOM 68 N GLY A 47 88.992 ATOM 69 CA GLY A 47 89.492 ATOM 69 CA GLY A 47 89.492 ATOM 60 CA GLY A 47 91.731 ATOM 61 CB GLY A 47 91.731 ATOM 62 CG GLY A 47 91.731 ATOM 63 CD GLY A 47 91.731 ATOM 64 CP CR 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46 83.801 24.083 ATOM 67 O GLN A 46 83.801 24.083 ATOM 68 N GLY A 47 88.992 23.042 ATOM 69 CA GLY A 47 89.492 22.066 ATOM 70 C GLY A 47 89.492 22.066 ATOM 71 O GLY A 47 91.005 21.903 ATOM 72 N PRO A 48 91.504 20.724 ATOM 73 CD PRO A 48 92.939 20.413 ATOM 76 CG PRO A 48 92.939 20.413 ATOM 77 C PRO A 48 92.939 20.413 ATOM 76 CG PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 92.949 18.883 ATOM 76 CG PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 92.949 18.883 ATOM 77 C PRO A 48 93.703 20.964 ATOM 78 O PRO A 48 93.703 20.964 ATOM 79 N ASP A 49 93.312 22.141 ATOM 79 N ASP A 49 93.991 22.755 ATOM 78 C PRO A 48 93.991 22.755 ATOM 78 C PRO A 49 93.991 22.755 ATOM 81 CB ASP A 49 95.381 23.259	ATOM 50 CA PRO A 44 90.930 23.899 -0.087 ATOM 51 CB PRO A 44 92.056 24.682 0.621 ATOM 52 CG PRO A 44 92.363 25.860 -0.251 ATOM 53 C PRO A 44 89.646 24.069 0.709 ATOM 54 O PRO A 44 88.967 25.089 0.591 ATOM 55 N GLY A 45 89.324 23.087 1.532 ATOM 56 CA GLY A 45 88.123 23.201 2.342 ATOM 57 C GLY A 45 89.460 24.624 3.724 ATOM 59 N GLN A 46 87.399 24.114 4.483 ATOM 59 N GLN A 46 87.399 24.114 4.483 ATOM 60 CA GLN A 46 87.570 24.868 5.729 ATOM 61 CB GLN A 46 85.157 24.661 6.612 ATOM 63 CD GLN A 46 85.157 24.661 6.612 ATOM 64 OE1 GLN A 46 85.143 25.874 8.699 ATOM 65 NE2 GLN A 46 85.143 25.874 8.699 ATOM 65 NE2 GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 66 C GLN A 46 88.053 23.908 6.822 ATOM 67 O GLN A 46 88.992 23.042 6.465 ATOM 68 N GLY A 47 88.992 23.042 6.465 ATOM 69 CA GLY A 47 88.992 23.042 6.465 ATOM 69 CA GLY A 47 89.492 22.066 7.410 ATOM 69 CA GLY A 47 89.492 22.066 7.410 ATOM 69 CA GLY A 47 91.005 21.903 7.413 ATOM 71 O GLY A 47 91.005 21.903 7.413 ATOM 72 N PRO A 48 91.504 20.724 6.987 ATOM 73 CD PRO A 48 92.939 20.413 6.984 ATOM 74 CA PRO A 48 92.939 20.413 6.984 ATOM 75 CB PRO A 48 92.939 20.413 6.984 ATOM 76 CG PRO A 48 92.939 20.413 6.984 ATOM 76 CG PRO A 48 92.939 20.413 6.984 ATOM 76 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ATOM 59 N GLY A 45 89.460 24.624 3.724 1.00 ATOM 59 N GLY A 46 87.399 24.114 4.483 1.00 ATOM 61 CB GLY A 46 87.399 24.126 </td

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	ATOM	84	OD2	ASP A	49	95.649	25.606	4.272	1.00 49.48
•	MOTA	85	С	ASP A	49	94.069	21.761	2.984	1.00 46.42
	ATOM	86	0	ASP A	49	93.071	21.119	2.667	1.00 47.58
•	ATOM	87	N	ARG A	50	95.245	21.636 -	2.353	1.00 43.75
5	ATOM	88	CA	ARG A	50	95.458	20.721	1.214	1.00 40.37
	MOTA	89	СВ	ARG A	50	95.508	19.239	1.659	1.00 41.78
	MOTA	90	CG	ARG A	50	94.176	18.621	2.058	1.00 44.71
	ATOM	91	CD	ARG A	50	93.970	17.261	1.398	1.00 47.92
	ATOM	92	NE	ARG A	、50	93.230	16.337	2.265	1.00 51.36
10	ATOM	93	CZ	ARG A	50	91.918	16.436	2.519	1.00 52.40
•	MOTA	94	NH1	ARG A	50	91.181	17.377	1.923	1.00 53.58
	ATOM	95	NH2	ARG A	50	91.343	15.589	3.368	1.00 52.49
	ATOM	96	Ċ	ARG A	50	94.437	20.938	0.092	1.00 36.07
	ATOM	97	0	ARG A	.50	93.374	20.329	0.054	1.00 34.88
15	ATOM	98	N	PRO A	51	94.760	21.823	-0.848	1.00 33.81
	MOTA	99	CD	PRO ·A	51	96.002	22.606	-0.891	1.00 34.21
	ATOM	100	CA	PRO A	51	93.879	22.123	-1.975	1.00 32.21
	MOTA	101	СВ	PRO A	51	94.686	23.116	-2.814	1.00 31.98
	ATOM	102	CG	PRO A	51	95.678	23.697	-1.870	1.00 32.93
20	MOTA	103	C	PRO P	A 51	93.569	20.878	-2.797	1.00 30.79
	MOTA	104	0	PRO P	A 51	94.436	20.049	-3.040	1.00 32.41
	MOTA	105	N	GLN A	A 52	92.327	20.768	-3.227	1.00 31.01
	ATOM	106	CA	GLN A	A 52	91.882	19.649	-4.038	1.00 31.10
	ATOM	107	CE	GLN A	A 52	91.036	18.656	-3.228	1.00 30.92
25	ATOM	108	s co	G GLN	A 52	89.656	19.164	-2.825	1.00 34.68
	MOTA	109	e CI	O GLN	A 52	89.132	18.495	-1.556	
	MOTA	110	0 01	E1 GLN	A 52	88.074	17.858	-1.561	1.00 38.16
•	ATOM	11:	L N	E2 GLN	A 52	89.874	18.637	-0.461	1.00 37.13
	MOTA	11:	2 C	GLN	A 52	91.108	3 20.158	-5.251	1.00 30.15
-30	ATOM	11	3 0	GLN	A 52	90.525	5 21.245	-5.221	1.00 29.33
	ATOM	11	4 N	GLU	A 53	91.09	9 19.367	-6.312	2 1.00 30.79
	ATOM	11	5 C	A GLU	A 53	90.38	3 19.740	-7.518	
	MOTA	11	.6 C	B GLU	A 53	90.83	7 18.877	-8.69	
	MOTA	11	.7 (G GLU	·A 53	91.68	0 19.628	-9.71	•
35	ATOM	11	.8 (CD GLU	A .53	92.67	5 18.733	-10.44	0 1.00 35.69

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	MOTA	119	OE1	GLU	A	53	93,828	19.181	-10.661	1.00	35.06
	ATOM	120	OE2	GLU	A	53	92.304	17.584	-10.781	1.00	35.68
	ATOM	121	C	GLU	A	53	88.880	19.615	-7.291	1.00	29.25
	ATOM	122	0	GLU	A	53	88.400	18.567	6.846	1.00	30.67
5	ATOM	123	N	VAL	A	54	88.148	20.697	-7.578	1.00	28.00
	MOTA	124	ĊA	VAL	A	54	86.695	20.739	-7.398	1.00	27.10
	ATOM	125	CB	VAL	A	54	86.281	21.745	-6.292	1.00	26.17
	MOTA	126	CG1	VAL	A	54	84.771	21.910	-6.253	1.00	23.81
	ATOM	127	CG2	VAL	A	54	86.805	21.294	-4.937	1.00	22.59
10	MOTA	128	C	VAL	A	54	86.001	21.113	-8.705	1.00	27.97
	ATOM	129	0	VAL	A	54	86.364	22.089	-9.359	1.00	28.40
	ATOM	130	N	SER	A	55	85.009	20.324	-9.082	1.00	27.75
	MOTA	131	CA	SER	A	55	84.281	20.564	-10.317	1.00	29.06
	ATOM	132	CB	SER	A	55	84.321	19.317	-11.212	1.00	27.82
-15	ATOM	133	OG	SER	A	55	85.649	18.850	-11.348	1.00	29.80
	ATOM	134	С	SER	A _.	55	82.845	20.965	-10.063	1.00	28.17
•	MOTA	135	0	SER	A	55	82.125	20.291	-9.322	1.00	28.82
	ATOM	136	N	TYR	A	56	82.434	22.052	-10.710	1.00	28.14
	MOTA	137	CA	TYR	A	56	81.073	22.558	-10.607	1.00	29.61
-20	MOTA	138	CB	TYR	A	56	80.969	23.720	-9.605	1.00	27.30
	MOTA	139	CG	TYR	A	56	81.822	24.941	-9.904	1.00	25.16
	MOTA	140	CD1	TYR	A	56	83.132	25.026	-9.443	1.00	25.56
	ATOM	141	CE1	TYR	A	56	83.905	26.154	-9.682	1.00	26.15
	ATOM	142	CD2	TYR	Ά	.56	81.308	26.021	-10.612	1.00	23.48
25	MOTA	143	CE2	TYR	A	56	82.073	27.149	-10.859	1.00	23.57
•	ATOM	144	CZ	TYR	A	56	83.370	27.210	-10.391	1.00	24:23
	MOTA	145	ОН	TYR	A	. 56	84.140	28.328	-10.636	1.00	27.89
•	MOTA	146	С	TYR	A	56	80.562	22.994	-11.972	1.00	31.23
	MOTA	147	0	TYR	A	56	81.354	23.278	-12.878	1.00	30.17
30	MOTA	148	N	THR	A	57	79.243	23.057	-12.107	1.00	33.31
	MOTA	149	CA	THR	A	57	78.620	23.476	-13.356	1.00	35.43
	MOTA	150	CB	THR	Α	57	78.412	22.276	-14.296	1.00	35.27
	ATOM	151	OG1	THR	A	57	77.984	22.698	-15.583	1.00	37.54
	ATOM	152	CG2	THR	. A	57	77.433	21.244	-13.785	1.00	33.54
35	ATOM	153	С	THR	A	57	77.310	24.215	-13.087	1.00	36.61

	MOTA	154	O	THR	A	57	7	6.936	24.426	-11.929	1.00	36.38
	ATOM	155	N	ASP	A	58	7	6.619	24.603	-14.163	1.00	36.33
	ATOM	156	.CA	ASP	A	58	7	5.347	25.315	-14.064	1.00	36.49
	ATOM	157	CB	ASP	A	58	7	4.297	24.467	-13.332	1.00	39.46
5	MOTA	158	CG	ASP	A	58	7	3.794	23.286	-14.157	1.00	41.91
	ATOM	159	OD1	ASP	A	58	7	3.025	22.461	-13.607	1.00	42.29
	MOTA	160	OD2	ASP	A	58	7	4.166	23.182	-15.352	1.00	44.17
	MOTA	161	C	ASP	A	58	7	5.513	26.673	-13.391	1.00	35.84
	ATOM	162	0	ASP	A	58	7	4.643	27.125	-12.655	1.00	34.21
10	MOTA	163	N	THR	A	59	7	6.639	27.312	-13.665	1.00	35.88
	MOTA	164	CA	THR	A	59	7	6.965	28.615	-13.114	1.00	37.28
	ATOM	165	CB	THR	A	59	7	8.403	28.955	-13.476	1.00	36.95
	ATOM	166	OG1	THR	A	59	7	9.257	27.884	-13.110	1.00	37.20
	ATOM	167	CG2	THR	A	59	7	18.930	30.221	-12.831	1.00	38.01
15	ATOM	168	С	THR	A	59	7	76.009	29.703	-13.596	1.00	38.01
	ATOM	169	0	THR	A	59	-	75.641	29.736	-14.767	1.00	39.28
	ATOM	170	N	LYS	A	60	•	75.613	30.597	-12.674	1.00	37.94
	ATOM	171	CA	LYS	A	60	•	74.704	31.698	-13.000	1.00	36.62
	MOTA	172	CB	LYS	A	60	•	73.259	31.196	-13.139	1.00	37.83
20	MOTA	173	·CG	LYS	A	60	•	72.517	31.015	-11.822	1.00	38.44
	MOTA	174	CD	LYS	A	60	•	71.034	31.300	-11.975	1.00	38.40
	MOTA	175	CE	LYS	A	60	•	70.199	30.076	-11.645	1.00	39.94
	MOTA	176	NZ	LYS	A	60	ı	68.909	30.441	-10.992	1.00	41.86
	ATOM	177	С	LYS	A	60		74.789	32.812	-11.957	1.00	36.32
25	MOTA	178	0	LYS	A	60	,	74.913	32.543	-10.768	1.00	36.41
	MOTA	179.	N	VAL	A	61		74.735	34.060	-12.421	1.00	34.99
	MOTA	180	CA	VAL	A	61		74.815	35.226	-11.555	1.00	33.46
	ATOM	181	CB	VAL	A	61		75.084	36.508	-12.368	1.00	34.41
	ATOM	182	CG1	VAL	A	61	•			-11.503	•	34.88
30	ATOM	183	CG2	2 VAL	, A	61		76.488	36.473	3 -12.970	1.00	33.02
	MOTA	184	С	VAL	A	6 <u>1</u>		73.536	35.386	5 -10.742	1.00	33.94
	MOTA	185	0	IAV	A	61		72.431	. 35.331	-11.295	1.00	31.92
	MOTA	186	N	ILE	E A	62		73.692	35.554	9.413		30.70
	ATOM	187	CA	ILE	E A	62		72.534	35.686	5 -8.518	1.00	30.06
35	MOTA	188	CB	ILE	E A	62		72.322	34.42	4 -7.649	1.00	31.30

	MOTA	189	CG2	ILE A	A	62	71.972	33.218	-8.511	1.00	29.51
	MOTA	190	CG1	ILE :	A	62	73.554	34.141	-6.777	1.00	29.23
	MOTA	191	CD1	ILE :	A	62	73.268	33.219	-5.610	1.00	31.27
	ATOM	192	C	ILE .	Α.	62	72.615	36.903	-7.602	1.00	28.13
5	MOTA	193	0	ILE .	A	62	71.629	37.255	-6.966	1.00	29.85
	MOTA	194	N	GLY .	A	63	73.773	37.546	-7.539	1.00	26.58
	MOTA	195	CA	GLY .	A	63	73.909	38.715	-6.696	1.00	26.14
	MOTA	196	С	GLY .	A	63	75.217	39.436	-6.899	1.00	27.79
	MOTA	197	0	GLY .	A	63	76.092	38.967	-7.627	1.00	29.41
10	ATOM	198	N	ASN	A	64	75.364	40.578	-6.249	1.00	27.39
	ATOM	199	CA	ASN	A	64	76.589	41.353	-6.362	1.00	28.10
٠.	ATOM	200	CB	ASN	A	64	76.724	41.953	-7.779	1.00	28.83
	ATOM	201	CG	ASN	A	64	75.706	43.040	-8.063	1.00	29.90
	ATOM	202	OD1	ASN	A	64	74.819	43.302	-7.253	1.00	32.34
15	ATOM	203	ND2	ASN	A	64	75.829	43.689	-9.220	1.00	31.39
	ATOM	204	С	ASN	A	64	76.656	42.451	-5.300	1.00	26.72
	ATOM	205	0	ASN	A.	64	75.726	42.639	-4.527	1.00.	27.02
	ATOM	206	N	GLY	A	65	77.759	43.177	-5.306	1.00	25.86
	ATOM	207	CA	GLY	A	65	77.975	44.267	-4.395	1.00	24.32
20	ATOM	208	С	GLY	A	65	79.267	44.955	-4.715	1.00	24.77
	ATOM	209	0	GLY	A	65	79.871	44.661	-5.747	1.00	22.63
	MOTA	210	N	SER	A	66	79.714	45.861	-3.838	1.00	23.92
	MOTA	211	CA	SER	A	66	80.968	46.573	-4.069	1.00	23.93
	MOTA	212	CB	SER	A	66	81.127	47.755	-3.102	1.00	28.01
25	ATOM	213	OG	SER	A	66	81.468	47.312	-1.792	1.00	33.78
	MOTA	214	С	SER	A	66	82.174	45.651	-4.006	1.00	21.75
	MOTA	215	0	SER	A .	66	83.293	46.050	-4.340	1.00	23.12
	ATOM	216	N	PHE	A	67	81.948	44.419	-3.576	1.00	21.22
	MOTA	217	CA	PHE	A	67	83.019	43.426	-3.459	1.00	21.95
30	MOTA	218	CB	PHE	A	67	82.635	42.390	-2.397	1.00	19.80
	MOTA	219	CG	PHE	A	67	81.371	41.638	-2.727	1.00	21.25
	ATOM	220	CD1	PHE	A	67	80.178	41.958	-2.107	1.00	21.15
	ATOM	.221	CD2	PHE	A	67	81.375	40.618	-3.677	1.00	21.87
	MOTA	222	CE1	PHE	A	67	79.014	41.285	-2.418	1.00	18.94
35	ATOM	223	CE2	PHE	A	67	80.217	39.940	-3.992	1.00	19.41

	ATOM	224	CZ	PHE	A	67	79.036	40.274	-3.361	1.00	21.96
	MOTA	225	C	PHE	A	67	83.241	42.684	-4.788	1.00	21.21
	ATOM	226	0	PHE	A	67	84.356	42.288	-5.117	1.00	21.27
	ATOM	227	N	GLY	A	68	82.154	42.459	-5.504	1.00	21.10
5	ATOM	228	CA	GLY	A	68	82.218	41.729	-6.744	1.00	19.70
	ATOM	229	C	GLY	A	68	80.882	41.159	-7.110	1.00	17.87
	MOTA	230	0	GLY	À	68	79.899	41.874	-7.159	1.00	21.48
	ATOM	231	N	VAL	A	69	80.841	39.876	-7.410	1.00	19.22
	ATOM	232	CA	VAL	A	69	79.590	39.262	-7.845	1.00	18.99
10	ATOM	233	CB	VAL	A	69	79.686	39.054	-9.385	1.00	20.73
	ATOM	234	CG1	VAL	A	69	78.464	38.338	-9.938	1.00	19.08
	MOTA	235	CG2	VAL	A	69	79.904	40.398	-10.058	1.00	20.67
	MOTA	236	С	VAL	A	69	79.371	37.914	-7.214	1.00	16.65
	ATOM	237	0	VAL	A	69	80.301	37.263	-6.861	1.00	17.62
15	MOTA	238	N	VAL	A	70	78.144	37.477	-7.124	1.00	17.29
	MOTA	239	CA	VAL	A	70	77.877	36.162	-6.558	1.00	19.87
	ATOM	240	CB	VAL	A	70	76.944	36.225	-5,328	1.00	19.21
	MOTA	241	CG1	VAL	A	70	76.827	34.839	-4.701 ·	1.00	16.63
-	MOTA	242	CG2	VAL	A	70	77.469	37.240	-4.317.	1.00	18.33
20	MOTA	243	С	VAL	Α.	70	77.286	35.217	-7.591	1.00	21.82
	MOTA	244	0	VAL	A	70	76.320	35.551	-8.255	1.00	22.52
	MOTA	245	N	TYR	A	71	77.875	34.032	-7.705	1.00	25.04
	MOTA	246	CA	TYR	. A	71	77.407	33.030	-8.657	1.00	28.92
	ATOM	247	СВ	TYR	A	71	78.603	32.453	-9.446	1.00	29.97
25	MOTA	248	CG	TYR	A	71	79.251	33.358	-10.469	1.00	33.56
	MOTA	249	CD1	TYR	A	71	78.711	33.511	-11.742	1.00	35.58
	MOTA	250	CE1	TYR	A	71	79.326	34.312	-12.693	1.00	36.15
	MOTA	251	CD2	TYR	A	71	80.426	34.033	-10.173	1.00	34.86
	ATOM	252	CE2	TYP	A S	71	81.045	34.843	-11.111	1.00	37.15
30	ATOM	253	CZ	TYF	R A	71	80.492	34.978	-12.372	1.00	37.44
	ATOM	254	OH	TYF	A S	71	81.117	35.771	-13.313	1.00	39.50
	ATOM	255	C	TYF	RA	71	76.746	31.838	-7.974	1.00	29.85
	ATOM	256	0	TY	R A	71	77.210	31.348	-6.942	1.00	29.76
	MOTA	257	N	GL	A R	72	75.736	31.294	-8.627	1.00	30.90
35	MOTA	258	CA	GL	A V	72	75.121	30.075	-8.154	1.00	31.38

	ATOM	259	СВ	GLN	A	72	73.616	30.050	-8.379	1.00	33.05
	ATOM ·	260	CG	GLN	A	72	72.915	28.963	-7.572	1.00	34.55
	MOTA	261	CD	GLN	A	72	71.721	28.374	-8.285	1.00	36.84
	MOTA	262	OE1	GLN	A	72	71.837	27.379	-9.001	1.00	37.72
5	MOTA	263	NE2	GLN	A	72	70.558	28.988	-8.092	1:00	39.46
	MOTA	264	C	GLN	A	72	75.792	28.950	-8.931	1.00	32.33
•	ATOM	265	0	GLN	A	72	76.249	29.163	-10.068	1.00	33.82
	MOTA	266	N	ALA	A	73	75.896	27.783	-8.332	1.00	31.53
	ATOM	267	CA	ALA	A	73	76.551	26.678	-8.998	1.00	31.65
10	ATOM	268	CB	ALA	A	73	78.061	26.826	-8.914	1.00	31.06
	ATOM	269	C	ALA	A	73	76.127	25.346	-8.426	1.00	32.36
	MOTA	270	0	ALA	A.	73	75.386	25.272	-7.447	1.00	31.34
	ATOM	271	N	LYS	A	74	76.618	24.295	-9.048	1.00	33.73
	ATOM	272	CA	LYS	A	74	76.324	22.956	-8.622	1.00	35.30
15	ATOM	273	СВ	LYS	A	74	75.177	22.372	-9.443	1.00	36.50
	ATOM	274	CG	LYS	A	74	74.794	20.960	-9.037	1.00	37.82
	ATOM	275	CD	LYS	A	74	73.610	20.453	-9.843	1.00	40.81
	ATOM	276	CE	LYS	A	74	74.036	19.415	-10.869	1.00	43.32
	ATOM	277	NZ	LYS	A	74	74.647	20.042	-12.078	1.00	46.77
20	ATOM	278	C	LYS	A	74	77.559	22.098	-8.760	1.00	36.85
	ATOM	279	0	LYS	A	74	78.124	21.975	-9.855	1.00	37.48
	ATOM	280	N	LEU	A	75	77.973	21.496	-7.648	1.00	37.35
	ATOM	281	CA	LEU	A	75 ·	79.131	20.622	-7.655	1.00	37.20
	ATOM	282	CB	LEU	A	75	79.586	20.322	-6.227	1.00	34.69
25	MOTA	283	CG	LEU	A	75	79.445	21.467	-5.222	1.00	34.55
	ATOM	284	CD1	LEU	A	75	79.241	20.922	-3.816	1.00	32.89
	ATOM	285	CD2	LEU	A	75	80.659	22.386	-5.276	1.00	31.32
	ATOM	286	С	LEU	A	75	78.747	19.333	-8.370	1.00	39.29
	ATOM	287	0	LEU	A	75	77.626	18.845	-8.213	1.00	38.83
30	ATOM	288	N	CYS	A	76	79.658	18.802	-9.174	1.00	41.06
	ATOM	289	CA	CYS	A	76	79.385	17.581	-9.928	1.00	43.45
	ATOM	290	CB	CYS	A	76	80.363	17.462	-11.094	1.00	42.71
	ATOM	291	SG	CYS	A	76	80.578	19.008	-12.012	1.00	42.33
	ATOM	292	С	CYS	A	76	79.442	16.345	-9.035	1.00	45.25
35	MOTA	293	0	CYS	A	76	78.682	15.392	-9.218	1.00	46.06

	ATOM	294	N	ASP	A	77	80.348	16.377	-8.072	1.00 4	7.16
	ATOM	295	CA	ASP	A	77	80.549	15.284	-7.128	1.00 4	9.51
	ATOM	296	СВ	ASP	A	77	81.638	15.664	-6.111	1.00 5	2.47
	ATOM	297	CG	ASP	A	77	81.672	17.160 .	-5.800	1.00 5	4.95
5	MOTA	298	OD1	ASP	A	77	80.869	17.607	-4.944	1.00 5	6.19
	MOTA	299	OD2	ASP	A	77 ·	82.499	17.885	-6.412	1.00 5	4.51
	ATOM	300	С	ASP	A	77	79.272	14.864	-6.392	1.00 4	9.21
•	ATOM	301	0	ASP	A	77	78.893	13.693	-6.415	1.00 4	9.89
	MOTA	302	N	SER	A	78	78.646	15.813	-5.699	1.00 4	8.59
10	ATOM	303	·CA	SER	. A	78	77.449	15.536	-4.899	1.00 4	7.33
	ATOM	304	СВ	SER	A	78	77.650	16.084	-3.482	1.00 4	7.77
	ATOM	305	OG	SER	A	78	78.037	17.452	-3.515	1.00 4	6.19
	MOTA	306	С	SER	A	78	76.170	16.125	-5.481	1.00 4	17.16
	MOTA	307	0	SEF	k A	78	75.074	15.833	-4.994	1.00 4	17.02
15	ATOM	308	N	GLY	'A	79	76.305	16.973	-6.496	1.00 4	16.01
	MOTA	309	CA	GLY	A	79	75.140	17.599	-7.084	1.00 4	43.58
	ATOM	310	С	GL)	Α	79	74.578	18.689	-6.191	1.00	42.64
	ATOM	311	0	GL:	Α	79	73.542	19.271	-6.495	1.00	42.66
	ATOM	312	N	GL	JA	80	75.265	18.955	-5.080	1.00	41.77
20	ATOM	313	CA	GL	JA	.80	74.845	19.969	-4.117	1.00	40.71
	ATOM	314	CB	GL	U A	80	75.661	19.856	-2.829	1.00	41.92
	ATOM	315	CG	GL	O A	80	75.323	18.632	-1.992	1.00	
	ATOM	316	CD	GL	U A	80	76.091	18.588	-0.684	1.00	47.47
	MOTA	317	OE	1 GL	U A	80	 77.297	18.258	-0.710		48.55
25	MOTA	318	OE	2 GL	U A	80	75.488	18.896	0.372		49.38
	ATOM	319	С	GL	U A	. 80	74.945	21.378	-4.695		39.89
	ATOM	320	0	GL	U A	80	75.796	21.659	-5.541		40.04
	ATOM	321	N	LE	U A	81	74.055	22.253	-4.237		38.33
	ATOM	322	CA	LE	U A	81	74.010	23.632	-4.701		36.18
30	ATOM	323	3 CE	3 LF	EU P	81	72.566	24.127	-4.728		36.89
	MOTA	324	C	G LI	EU P	81	71.763	23.803	-5.984		37.28
	ATOM	325	5 CI	Ol LI	EU A	81	71.712	22.303	-6.209		38.67
	ATOM	326	6 CI)2 L	EU A	A 81	70.360	24.379	-5.877		38.16
	MOTA	32	7 C	L	EU A	A 81	74.840	24542	-3.812		34.75
35	MOTA	328	8 0	L	EU J	A 81	74.720	24.506	-2.585	1.00	36.28

	ATOM	329	N	VAL A	8	32	75.675	25.363	-4.434	1.00	31.15
	ATOM	330	CA	VAL A	8	32	76.514	26.287	-3.694	1.00	28.31
	ATOM	331	CB	VAL A	8	32	78.001	25.855	-3.667	1.00	29.78
	ATOM	332	CG1	VAL A	8	32 .	78.211	24.602	2.825	1.00	29.34
5	ATOM	333	CG2	VAL A	8	32	78.554	25.671	-5.081	1.00	30.69
	ATOM	334	С	VAL A	8	32 .	76.450	27.678	-4.290 ·	1.00	27.28
	MOTA	335	0	VAL A	8	32	75.925	27.892	-5.400	1.00	25.63
-	ATOM	336	N	ALA A	8	33	77.030	28.607	-3.557	1.00	22.81
	ATOM	337	CA	ALA A	8	33	77.127	29.975	-3.976	1.00	20.75
10	ATOM	338	СВ	ALA A	8	33	76.304	30.895	-3.090	1.00	19.91
	ATOM	339	С	ALA A	8	33	78.594	30.325	-3.953	1.00	20.33
	ATOM	340	0	ALA A	8	33	79.320	29867	-3.068	1.00	20.70
	ATOM	341	N.	ILE A	8	34	79.040	31.088	-4.944	1.00	19.79
	MOTĄ	342	CA	ILE A	8	34	80.441	31.476	-5.066	1.00	19.64
15	ATOM	343	CB	ILE A	8	3 4	81.101	30.853	-6.331	1.00	19.52
	ATOM	344	CG2	ILE A	. 8	34	82.608	31.066	-6.319	1.00	16.65
	ATOM	345	CG1	ILE A	8	3 4	80.758	29.358	-6.423	1.00	16.97
	ATOM	346	CD1	ILE A	8	3 4	81.795	28.503	-7.134	1.00	21.03
	ATOM	347	С	ILE A	8	3 4	80.538	32.992	-5.093	1.00	22.12
20	ATOM	348	0	ILE A	8	34	80.055	33.621	-6.031	i.00	22.68
	ATOM	349	N	LYS A	8	35	81.111	33.562	-4.017	1.00	22.75
	ATOM	350	CA	LYS A	8	35	81.224	35.008	-3.844	1.00	24.97
	ATOM	351	CB	LYS A	8	35	81.564	35.333	-2.383	1.00	25.35
	ATOM	352	CG	LYS A	8	35	81.822	36.803	-2.115	1.00	25.03
25	ATOM	353	CD	LYS A	8	35	80.620	37.460	-1.467	1.00	27.75
	ATOM	354	CE	LYS A	8	35	80.832	37.658	0.027	1.00	28.19
	ATOM	355	NZ	LYS A	8	35	81.048	39.089	0.363	1.00	29.61
	MOTA	356	С	LYS A	8	35	82.218	35.695	-4.791	1.00	27.05
•	ATOM	357	0	LYS A	8	35	81.868	36.659	-5.418	1.00	30.22
30	ATOM	358	N	LYS A	8	36	83.445	35.243	-4.901	1.00	27.41
	ATOM	359	CA	LYS A	8	36	84.405	35.914	-5.825	1.00	28.29
	ATOM	360	CB	LYS A	. 8	36	83.963	35.770	-7.294	1.00	27.88
	ATOM	361	CG	LYS A	. 8	36	84.896	36.486	-8.266	1.00	29.66
	MOTA	362	CD	LYS A	. 8	36	84.710	35.997	-9.700	1.00	30.66
35	ATOM	363	CE	LYS A	. 8	36	85.545	36.801	-10.683	1.00	31.77

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	ATOM	364	NZ	LYS	A	86	85.528	36.200	-12.056	1.00 3	3.13
	ATOM	365	С	LYS	A	86	84.583	37.403	-5.528	1.00 2	5.91
	ATOM	366	0	LYS	A	86	83.726	38.224	-5.827	1.00 2	25.06
	ATOM	367	N	VAL	A	87	85.710	37.753	4.960	1.00 2	26.67
5	ATOM	368	CA	VAL	A	87	85.975	39.138	-4.643	1.00 2	28.24
	ATOM	369	СВ	VAL	A	87	. 85.798	39.421	-3.124	1.00 2	29.12
	ATOM	370	CG1	VAL	A	87	84.605	38.644	-2.574	1.00 2	27.52
	ATOM	371	CG2	VAL	A	87	87.060	39.068	-2.347	1.00 2	29.13
	MOTA	372	С	VAL	A	87	87.368	39.530	-5.085	1.00 2	29.97
10	ATOM	373	0	VAL	A	87	88.314	38.771	-4.931	1.00 2	29.26
	ATOM	374	N	LEU	A	88	87.484	40.724	-5.627	1.00	33.85
	ATOM	375	CA	LEU	A	88	88.764	41.230	-6.077	1.00	37.36
	ATOM	.376	CB	LEU	A	88	88.559	42.551	-6.820	1.00	36.76
	MOTA	377	CG	LEU	A	88	89.821	43.234	-7.336	1.00	37.85
15	MOTA	378	CD1	LEU	Ä	88	90.512	42.365	-8.371	1.00	37.97
	MOTA	379	CD2	LEU	A	88	89.490	44.606	-7.899	1:00	37.34
	ATOM	380	С	LEU	A	88	89.664	41.417	-4.863	1.00	40.30
	MOTA	381	0	LEU	A	88	89.382	42.246	-3.994	1.00	40.89
	MOTA	382	N	GLN	A	89	90.717	40.606	-4.784	1.00	43.74
20	ATOM	383	CA	GLN	A	89	91.636	40.638	-3°. 653	1.00	46.09
	MOTA	384	CB	GLN	A	89	91.929	39.211	-3.181	1.00	45.39
	MOTA	385	, CG	GLN	A	89	91.367	38.863	-1.809	1.00	46.90
	MOTA	386	CD	GLN	Α	89	91.570	39.957	0.778	1.00	46.72
	MOTA	387	OE1	GLN	Α	89	90.604	40.507	-0.250	1.00	47.40
25	ATOM	388	NE2	GLN	Α	89	92.828	40.277	-0.484	1.00	47.16
	ATOM	389	С	GLN	IA	89	92.949	41.333	-3.983	1.00	47.93
	MOTA	390	0	GLN	I A	89	93.489	41.181	-5.082	1.00	49.02
	MOTA	391	N	ASE	A	90	93.474	42.061	-2.996	1.00	49.68
	MOTA	392	CA	ASI	? A	90	94.747	42.759	-3.116	1.00	51.13
30	MOTA	393	. CB	ASI	? A	90	94.751	43.989	-2.193	1.00	51.29
	MOTA	394	CG	ASI	? A	90	95.927	44.936	-2.407	1.00	50.48
	ATOM	395	OD:	1 AS	P A	90	97.031	44.464	-2.756		50.57
	ATOM	396	OD:	2 AS	P A	90	95.743	46.157	7 -2.211		50.42
	ATOM .	397	С	AS	P A	90	95.878	41.807	7 -2.718		53.33
35	ATOM	398	0	AS	P A	90	95.963	41.39	1 -1.555	1.00	53.28

	ATOM	399	N	LYS	A	91	96.729	41.446	-3.691	1.00	54.33
	ATOM	400	CA	LYS	A	91	97.850	40.525	-3.443	1.00	55.74
	ATOM	401	CB	LYS	A	91	98.910	40.577	-4.565	1.00	56.05
	ATOM	402	CG	LYS	A	91	98.677	41.643	-5.628	1.00	56.67
5	MOTA	403	CD	LYS	A	91	99.989	42.181	-6.181	1.00	56.82
	ATOM'	404	CE	LYS	A	91	99.975	43.703	-6.266	1.00	56.25
	MOTA	405	NZ	LYS	A	91	101.277	44.307	-5.849	1.00	55.53
	ATOM	406	С	LYS	A	91	98.519	40.811	-2.097	1.00	56.53
	MOTA	40.7	0	LYS	A	91	98.699	41.971	-1.713	1.00	56.04
10	ATOM	408	N	ARG	A	92	98.870	39.734	-1.389	1.00	57.95
	ATOM	409	CA	ARG	A	92	99.509	39.812	-0.070	1.00	59.85
	ATOM	410	CB	ARG	A	92	101.031	39.971	-0.194	1.00	61.28
	ATOM	411	CG	ARG	A	92	101.765	39.884	1.149	1.00	63.11
٠	ATOM	412	CD	ARG	A	92	101.170	38.809	2.066	1.00	64.33
15	MOTA	413	NE	ARG	A	92	101.534	37.450	1.636	1.00	65.78
	MOTA	414	CZ	ARG	A	92	102.171	36.543	2.403	1.00	66.33
	MOTA	415	NHl	ARG	A	92	102.468	36.805	3.681	1.00	65.70
	MOTA	416	NH2	ARG	A	92	102.504	35.359	1.886	1.00	66.03
	MOTA	417	С	ARG	A	92	98.920	40.936	0.787	1.00	59.66
20	MOTA	418	0	ARG	A	92	99.505	42.015	0.933	1.00	60.23
	MOTA	419	N	PHE	A	93	97.761	40.655	1.359	1.00	59.03
	ATOM	420	CA	PHE	A	93	97.053	41.589	2.223	1.00	57.37
	ATOM	421	CB	PHE	A	93	96.307	42.649	1.414	1.00	58.54
	MOTA	422	CG	PHE	A	93	96.818	44.050	1.630	1.00	59.76
25	ATOM	423	CD1	PHE	A.	93	98.128	44.276	2.024	1.00	59.99
	ATOM	424	CD2	PHE	A	93	95.989	45.141	1.436	1.00	59.95
	ATOM	425	CE1	PHE	A	93	98.600	45.559	2.219	1.00	60.16
	ATOM	426	CE2	PHE	A	93	96.454	46.427	1.630	1.00	60.63
	ATOM	427	CZ	PHE	A	93	97.762	46.637	2.021	1.00	60.34
30	ATOM	428	С	PHE	Α	93	96.105	40.830	3.141	1.00	55.64
	MOTA	429	0	PHE	A	93	95.906	41.237	4.294	1.00	57.05
	ATOM	430	N	LYS	A	94	95.528	39.703	2.659	1.00	52.25
	ATOM	431	CA	LYS	A	94	94.726	38.799	3.520	1.00	48.57
	ATOM	432	CB	LYS	A	94	95.291	38.777	4.945	1.00	49.85
35	ATOM	433	CG	LYS	A	94	96.746	38.348	5.024	1.00	50.64

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	ATOM	434	CD	LYS	A	94	96.932	37.126	5.901	1.00 5	2.78
	MOTA	435	CE	LYS	A	94	97.476	35.949	5.095	1.00 5	3.32
	ATOM	436	NZ	LYS	A	94	98.246	35.007	5.950	1.00 5	5.33
	ATOM	437	С	LYS	A	94	93.225	39.165 .	3.655	1.00 4	4.61
5	ATOM	438	0	LYS	A	94	92.892	40.177	4.271	1.00 4	5.08
	MOTA	439	N	ASN	A	95	92.349	38.387	3.103	1.00 4	0.22
	ATOM	440 .	CA	ASN	A	95	90.951	38.674	3.184	1.00 3	6.27
	MOTA	441	СВ	ASN	A	95	90.209	37.784	2.208	1.00 3	32.62
	ATOM	442	CG	ASN	A	95	88.768	38.190	1.998	1.00.3	32.71
10.	ATOM	443	OD1	ASN	A	95 .	87.870	37.731	2.709	1.00 3	32.10
	ATOM	444	ND2	ASN	A	95	88.531	39.051	1.011	1.00 3	33.84
	MOTA	445	С	ASN	A	95	90.380	38.559	4.600	1.00 3	33.71
	ATOM	446	0	ASN	A	95	90.540	37.518	5.237	1.00 3	32.21
	ATOM	447	Ŋ	ARG	A	96	89.731	39.618	5.080	1.00 3	31.07
15	ATOM	448	CA	ARG	A	96	89.146	39.634	6.408	1.00 2	28.30
	ATOM	449	СВ	ARG	A	96	88.612	41.034	6.729	1.00 2	28.81
	ATOM	450	CG	ARG	A	96	88.371	41.285	8.216	1.00 2	27.99
	ATOM	451	CD	ARG	A	96	89.015	42.582	8.681	1.00 2	28.70
	ATOM	452	NE	ARG	Ą	96	88.085	43.704	8.620	1.00	28.92
20	ATOM	453	CZ	ARG	A	96	88.421	44.970	8.882	1.00	29.89
	ATOM	454	NH1	ARG	A	96	89.652	45.280	9.267	1.00	33.01
	MOTA	455	NH2	ARG	A	96	87.521	45.930	8.775	1.00	31.42
	ATOM	456	С	ARG	A	96	88.031	38.615	6.512	1.00	
	MOTA	457	0	ARC	A	96	87.986	37.816	7.459	1.00	28.68
25	MOTA	458	N	GLU	JA	97	87.124	38.644	5.534	1.00	25.77
	ATOM	459	CA	GLU	JA	97	85.994	37.730	5.507	1.00	22.33
	ATOM	460	CB	GL	JA	97	85.089	38.035	4.313	1.00	24.09
	ATOM	461	CG	GL	JA	97	83.803	37.214	4.227	•	21.86
	ATOM	462	CD	GL	JA	· 97	82.859	37.724	3.140	1.00	21.24
30	MOTA	463	OE!	l GL	AU	97	81.665	37.342	3.150		19.24
	ATOM	464	OE2	2 GL	U A	97	83.314	38.514	2.284	1.00	21.60
	MOTA	465	С	GL	A U	97	86.425	36.271	5.528	.1.00	21.90
	MOTA	466	0	GL	A U	97	85.815	35,451	6.219	1.00	24.32
t	ATOM	467	N	LE	A U	. 98	87.469	35.939	4.773	1.00	20.92
35	ATOM	468	CA	LE	U A	. 98	87.959	34.559	4.710	1.00	20.46

	MOTA	469	CB	LEU	A	98	89.002	34.374	3.610	1.00	17.45
	MOTA	470	CG	LEU	A	98	89.629	32.987	3.552	1.00	15.40
	ATOM	471	CD1	LEU	A	98	88.569	.31.936	3.258	1.00	14.25
	ATOM	472	CD2	LEU	A	98	90.749	32.941	2.521	1.00	20.54
5	ATOM	473	С	LEU	A	98	88.532	34.070	6.043	1.00	20.25
	MOTA	474 .	0	LEU	A	98	88.311	32.923	6.428	1.00	17.48
	MOTA	475	N	GLN	A	99	89.280	34.937	6.719	1.00	21.83
	ATOM	476	CA	GLN	A	99	89.890	34.584	7.996	1.00	25.86
	MOTA	477	CB	GLN	A	99	90.957	35.602	8.415	1.00	28.40
10	MOTA	478	CG	GLN	A	99	`92.051	35.830	7.369	1.00	34.01
	MOTA	479	CD	GLN	A	99	92.960	34.619	7.138	1.00	38.37
	ATOM	480	OE1	GLN	A	99	94.019	34.487	7.763	1.00	40.68
	MOTA	481	NE2	GLN	A	99	92.562	33.738 [.]	6.219	1.00	39.28
	ATOM	482	C	GLN	A	99	88.826	34.362	9.079	1.00	23.77
15	ATOM	483	Ô	GLN	A	99	88.952	33.458	9.892	1.00	26.29
	ATOM	484	N	ILE	A,	100	87.753	35.154	9.036	1.00	24.72
	ATOM	485	CA	ILE	A	100	86.634	35.019	9.972	1.00	22.35
	MOTA	486	CB	ILE	A	100	85.700	36.249	9.914	1.00	18.73
	MOTA	48.7	CG2	ILE	A	100	84.337	35.943	10.530	1.00	17.79
20	ATOM	488	CG1	ILE	A	100	86.352	37.446	10.607	1.00	17.16
	ATOM	489	CD1	ILE	A	100	85.569	38.738	10.478	1.00	18.68
	ATOM	490	C _.	ILE	A	100	85.820	33.758	9.676	1.00	25.52
	MOTA	491	0	ILE	A	100	85.448	33.023	10.596	1.00	26.11
	ATOM	492	Ν.	MET	A	101	85.533	.33:523	8.383	1.00	25.86
25	ATOM .	493	CA	MEŢ	A	101	84.746	32.368	7.930	1.00	25.27
	ATOM	494	CB	MET	A	101	84.471	32.467	6.426	1.00	29.17
	MOTA	495	CG	MET	A	101	83.524	33.583	6.040	1.00	27.98
	MOTA	496	SD	MET	A	101	81.810	33.114	6.260	1.00	36.43
	MOTA	497	CE	MET	A	101	81.013	34.091	4.977	1.00	35.05
30	ATOM	498	C	MET	A	101	85.404	31.024	8.243	1.00	25.14
	MOTA	499	0	MET	A	101	84.729	30.062	8.618	1.00	25.95
	ATOM	500	N	ARG	A	102	86.713	30.954	8.080	1.00	25.37
	MOTA	501	CA	ARG	A	102	87.454	29.725	8.346	1.00	27.16
	ATOM	502	CB	ARG	A	102	88.897	29.893	7.896	1.00	27.85
35	ATOM	503	CG	ARG	A	102	89.101	29.711	6.405	1.00	31.76

	ATOM	504	CD	ARG A	102	90.344	28.885	6.123	1.00 3	0.40
	ATOM	505	NE	ARG A	102	91.474	29.723	5.762	1.00 3	2.24
	MOTA	506	CZ	ARG A	102	92.682	29.251	5.484	1.00 3	1.50
	MOTA	507	NHl	ARG A	102	92.924	27.946	5.561	1.00 3	3.59
5	ATOM	508	NH2	ARG A	102	93.653	30.085	5.129	1.00 3	3.23
	ATOM	509	С	ARG A	102	87.418	29.321	9.842	1.00 2	7.31
	ATOM	510	0	ARG A	102	87.675	28.167	10.172	1.00 2	7.37
	MOTA	511	N	LYS A	. 103	87.108	30.267	10.735	1.00 2	7.43
	MOTA	512	CA	LYS A	103	87.057	29.982	12.171	1.00 2	8.05
10	MOTA	513	CB	LYS A	103	87.529	31.193	12.978	1.00 2	28.46
	MOTA	514	CG	LYS A	103	88.957	31.618	12.690	1.00 2	28.79
	MOTA	515	.CD	LYS A	103	89.201	33.055	13.123	1.00 3	33.11
	ATOM	516	CÈ	LYS F	103	88.674	33.318	14.527	1.00 3	34.14
	MOTA	517	NZ	LYS F	103	89.068	34.665	15.016	1.00 3	35.09
15	ATOM .	518	С	LYS A	103	85.656	29.608	12.647	1.00 2	
	MOTA	519	0	LYS A	A 103	85.500	29.105	13.761	1.00 2	27.60
	MOTA	520	N	LEU A	A 104	84.645	29.882	11.832	1.00	24.89
	MOTA	521	CA	LEU A	A 104	83.270	29.602	12.209	1.00	24.18
	ATOM	522	CB	LEU I	A 104	82.322	30.650	11.619	1.00	24.18
20	MOTA	523	CG	LEU 3	A 104	82.703	32.114	11.872	1.00	24.11
	MOTA	524	CD:	LEU.	A 104	81.625	33.052	11.347	1.00	21.41
	ATOM	525	CD	2 LEU.	A 104	82.958	32.354	13.359	1.00	23.00
	MOTA	526	C	LEU	A 104	82.804	28.201	11.838	1.00	26.40
	MOTA	527	0	LEU	A 104	83.179	27.653	10.789	1.00	26.85
25	MOTA	528	N	ASP	A 105	81.947	27.648	12.705	1.00	23.78
	ATOM	529	CA	ASP	A 105	81.353	26.331	12.533		22.44
	MOTA	530	CB	ASP	A 105	82.361	25.215	12.822		23.57
	MOTA	531	CG	ASP	A 105	81.780	23.820	12.627		23.62
	ATOM	532	O	1 ASP	A 105	80.616	23.699	12.193		28.28
30	ATOM	533	OI	2 ASP	A 105	82.487	22.847	12.911	1.00	28.66
	MOTA	534	C	ASP	A 105	80.127	7 26.195	13.426		23.03
	MOTA	535	5 0	ASP	A 105	80.180	25.590	14.497	1.00	24.10
	MOTA	536	6 N	HIS	A 106	79.030	26.779	12.981	•	23.13
	ATOM	53	7 C	A HIS	A 106	77.78	6 26.763	3 13.712		22.25
35	MOTA	53	8 C	B HIS	A 106	77.57	0 28.132	14.339	1.00	23.75

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	ATOM	539	CG	HIS	A	106	76.513	28.159	15.391	1.00	24.95
	ATOM	540	CD2	HIS	A	106	76.590	27.976	16.734	1.00	25.19
	ATOM	541	ND1	HIS	A	106	75.194	28.434	15.118	1.00	25.11
	ATOM	542	CE1	HIS	A	106	74.500	28.427	16.245	1.00	27.00
5	ATOM	543	NE2	HIS	A	106	75.326	28.151	17.238	1.00	23.85
	ATOM	544	C	HIS	A	106	76.613	26.415	12.801	1.00	24.48
	MOTA	545	0	HIS	A	106	76.613	26.757	11.616	1.00	25.58
	ATOM	546	N	CYS	A	107	75.617	25.729	13.367	1.00	24.64
	ATOM	547	CA	CYS	A	107	74.425	25.300	12.644	1.00	25.69
10.	MOTA	548	CB	CYS	A	107	73.612	24.293	13.478	1.00	28.55
•	ATOM	549	SG	CYS	A	107	72.821	24.992	14.957	1.00	36.02
	ATOM	550	С	CYS	A	107	73.538	26.451	12.181	1.00	24.85
	ATOM	551	0	CYS	A	107	72.648	26.245	11.355	1.00	24.42
	ATOM	552	N	ASN	A	108	73.773	27.658	12.705	1.00	23.50
15	MOTA	553	CA	ASN	A	108	72.974	28.824	12.316	1.00	21.14
	ATOM	554	CB	ASN	A	108	72.246	29.457	13.506	1.00	23.02
	MOTA	555	CG	ASN	A	108	71.268	28.512	14.168	1.00	23.46
	ATOM	556	OD1	ASN	A	108	71.408	28.178	15.358	1.00	25.29
	ATOM	557	ND2	ASN	A	108	70.274	28.073	13.414	1.00	22.20
20	MOTA	558	C	ASN	A	108	73.807	29.861	11.571	1.00	18.73
	ATOM	559	0	ASN	A	108	73.453	31.030	11.521	1.00	18.69
	MOTA	560	N	ILE	A	109	74.898	29.410	10.971	1.00	20.13
	ATOM	561	CA	ILE	A	109	75.785	30.267	10.184	1.00	20.40
	ATOM	562	CB	ILE	A	109	77.101	30.556	10.918	1.00	20.32
25	ATOM	563	CG2	ILE	A	109	78.010	31.422	10.052	1.00	18.74
	ATOM	564	CG1	ILE	A	109	76.842	31.217	12.291	1.00	19.54
	ATOM	565	CD1	ILE	A	109	78.073	31.857	12.894	1.00	15.97
	ATOM	566	С	ILE	A	109	76.119	29.566	8.858	1.00	21.15
	ATOM .	567	0	ILE	A	109	76.427	28.366	8.853	1.00	20.11
30	ATOM	568	N	VAL	A	110	76.056	30.305	7.733	1.00	21.78
	MOTA	569	CA	VAL	Ą	110	76.366	29.707	6.412	1.00	21.66
	MOTA	570	CB	VAL	A	110	76.168	30.692	5.227	1.00	-22.90
	MOTA	571	CG1	VAL	A	. 110	77.375	31.600	5.048	1.00	22.85
	MOTA	572	CG2	VAL	A	. 110	75.891	29.918	3.949	.1.00	26.40
35	ATOM	573	С	VAL	A	110	77.773	29.149	6.401	1.00	19.25

	ATOM	574	0	VAL A	110	78.722	29.842	6.746	1.00	19.84
	ATOM	575	N	ARG A	111	77.894	27.886	6.036	1.00	19.86
	ATOM	576	CA	ARG A	111	79.184	27.207	6.015	1.00	21.87
	MOTA	577	CB	ARG A	111	78.955	25.702	6.024	1.00	24.97
5	ATOM	578	CG	ARG A	111	80.229	24.888	6.100	1.00	29.38
•	ATOM	579	CD	ARG A	111	79.924	23.401	6.091	1.00	34.23
	MOTA	580	NE .	ARG A	111	81.103	22.604	5.751	1.00	37.78
	ATOM	581	CZ	ARG A	111	81.057	21.418	5.144	1.00	40.20
	ATOM	582	NH1	ARG A	111	79.890	20.865	4.812	1.00	41.37
10	ATOM	583	NH2	ARG A	111	82.190	20.783	4.858	1.00	43.22
	MOTA	584	С	ARG A	111	80.053.	27.564	4.797	1.00	23.84
	ATOM	585	Ο.	ARG A	111	79.553	27.707	3.677	1.00	24.32
	ATOM	586	N	LEU A	112	81.366	27.646	5.044	1.00	22.96
	MOTA	587	CA	LEU A	112	82.370	27.918	4.031	1.00	22.62
15	ATOM	588	CB	LEU A	112	83.455	28.848	4.578	1.00	20.55
	ATOM	589	CG	LEU A	112	84.707	29.053	3.717	1.00	22.70
	ATOM	590	CD1	LEU A	112	84.370	29.778	2.415	1.00	23.13
	ATOM	591	CD2	LEU A	112	85.769	29.814	4.495	1.00	21.66
	MOTA	592	С	LEU A	112	82.962	26.582	3.569	1.00	23.22
20	ATOM	593	0	LEU A	112	83.854	26.014	4.207	1.00	22.92
	ATOM	594	N	ARG A	113	82.416	26.075	2.467	1.00	22.08
	ATOM	595	CA	ARG A	113	82.833	24.794	1.902	1.00	20.00
	ATOM	596	CB	ARG A	113	81.864	24.373	0.813	1.00	22.28
	ATOM	597	CG	ARG A	113	80.425	24.419	1.254	1.00	22.76
25	ATOM	598	CD	ARG A	113	79.947	23.054	1.678	1.00	28.44
	MOTA	599	NE	ARG A	113	78.566	22.834	1.271	1.00	32.49
	ATOM	600	CZ	ARG A	113	78.119	21.724	0.683	1.00	33.10
	ATOM	601	NH1	ARG A	. 113	78.949	20.723	0.386.	1.00	33.75
	MOTA	602	NH2	ARG A	. 113	76.831	21.621	0.392	1.00	35.17
30	ATOM	603	С	ARG A	. 113	84.231	24.840	1.343	1.00	16.86
	ATOM	604	0	ARG A	. 113	85.025	23.938	1.578	1.00	15.68
	ATOM	605	N	TYR A	114	84.527	25.889	0.590	1.00	19.17
	ATOM	606	CA	TYR A	114	85.845	26.044	-0.014	1.00	16.95
	ATOM	607	CB	TYR A	114	85.930	25.304	-1.371	1.00	18.87
35	ATOM	608	CG	TYR A	114	85.644	23.829	-1.394	1.00	15.79

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		ATOM	609	CD1	TYR A	114	84.377	23.365	-1.646	1.00	18.97
		ATOM	610	CE1	TYR A	114	84.114	22.014	-1.686	1.00	20.84
	•	ATOM	611	CD2	TYR A	114	86.655	22.905	-1.187	1.00	18.92
		ATOM	612	CE2	TYR A	114	86.404	21.558 .	-1.224	1.00	18.34
	5	ATOM	613	CZ.	TYR A	114 .	85.133	21.119	-1.474	1.00	21.38
		MOTA	614	ОН	TYR A	114	84.871	19.769	-1.505	1.00	26.51
		ATOM	615	C	TYR A	114	86.124	27.494	-0.331	1.00	15.53
		ATOM	616	0	TYR A	114	85.227	28.321	-0.402	1.00	17.41
•		ATOM	617	N .	PHE A	115	87.371	27.749	-0.627	1.00	16.85
	10	ATOM	618	CA	PHE A	115	87.826	29.043	-1.072	1.00	20.16
		ATOM	619	CB	PHE A	115	88.345	29.934	0.064	1.00	18.14
		ATOM	620	CG	PHE A	115	89.569	29.436	0.771	1.00	18.65
	·	ATOM	621	CD1	PHE A	115	90.822	29.914	0.432	1.00	19.77
		ATOM	622	CD2	PHE A	115	89.467	28.512	1.798	1.00	20.84
	15	MOTA	623	CE1	PHE A	115	91.952	29.475	1.101	1.00	22.37/
		ATOM	624	CE2	PHE A	115	90.589	28.070	2.465	1.00	19.43
		MOTA	625	CZ	PHE A	. 115	91.832	28.550	2.119	1.00	20.49
		ATOM	626	С	PHE A	115	88.881	28.806	-2.149	1.00	20.03
		MOTA	627	0	PHE A	. 115	89.624	27.837	-2.078	1.00	18.98
	20	MOTA	628	N	PHE A	116	88.930	29.656	-3.157	1.00	23.37
		ATOM	629	CA	PHE A	. 116 .	89.909	29.462	-4.232	1.00	22.44
	•	MOTA	630	CB	PHE A	. 116	89.464	28.335	-5.170	1.00	22.20
		MOTA	631	CG	PHE A	116	88.290	28.662	-6.050	1.00	22.32
	•	ATOM	632	CD1	PHE A	116	88.483	29.271	-7.290	1.00	22.41
	25	MOTA	633	CD2	PHE A	116	87.007	28.335	-5.662	1.00	19.00
		ATOM	634	CE1	PHE A	116	87.412	29.547	-8.124	1.00	22.74
		MOTA	635	CE2	PHE A	116	85.929	28.609	-6.485	1.00	24.32
		MOTA	636	CZ	PHE A	116	86.131	29.216	-7.726	1.00	21.99
		MOTA	637	С	PHE A	116	90.167	30.739	-4.993	1.00	23.65
	30	MOTA	638	. 0	PHE A	116	89.309	31.614	-5.067	1.00	23.70
		MOTA	639	N	TYR A	A 117	91.360	30.850	-5.543	1.00	27.46
		ATOM	640	CA	TYR A	A 117	91.744	32.035	-6.283	1.00	31.04
		MOTA	641	СВ	TYR A	A 117	93.154	32.450	-5.907	1.00	30.88
		ATOM	642	CG	TYR A	A 117	93.281	32.754	-4.432	1.00	30.90
	35	ATOM	643	CD1	TYR A	A 117	93.589	31.754	-3.526	1.00	30.87
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	ATOM	644	CE1	TYR A	117	93.708	32.024	-2.175	1.00	31.90
	MOTA	645	CD2	TYR A	117	93.089	34.036	-3.950	1.00	30.52
	MOTA	646	CE2	TYR A	117	93.203	34.319	-2.602	1.00	32.72
	ATOM	647	CZ	TYR A	117	93.515	33.307	1.718	1.00	32.15
5	ATOM	648	ОН	TYR A	117	93.647	33.582	-0.381	1.00	31.58
	MOTA	649	С	TYR A	117	91.570	31.864	-7.786	1.00	33.82
	ATOM	650	0	TYR A	117	91.556	30.744	-8.299	1.00	34.45
	MOTA	651	N	SER A	118	91.406	32.993	-8.473	1.00	37.08
	ATOM	652	CA	SER A	118	91.200	33.024	-9.921	1.00	39.93
10	ATOM .	653	СВ	SER A	118	89.703	32.964	-10.247	1.00	38.74
	MOTA	654	OG	SER A	118	89.054	34.178	-9.909	1.00	37.18
	ATOM	655	C	SER A	118	91.838	34.274	-10.531	1.00	42.40
	ATOM	656	0	SER A	118	92.023	35.278	-9.849	1.00	42.03
	ATOM	657	N	SER A	119	92.198	34.195	-11.810	1.00	46.22
15	MOTA	658	CA	SER A	119	92.852	35.316	-12.492	1.00	50.06
	ATOM	659	CB	SER A	119	94.035	34.802	-13.326	1.00	50.24
	ATOM	660	OG	SER A	119	94.416	33.499	-12.924	1.00	50.86
	ATOM	661	C	SER A	119	91.910	36.117	-13.385	1.00	52.37
	ATOM	662	0	SER A	119	91.903	37.347	-13.341	1.00	52.91
20	MOTA	663	N	GLY A	120	91.130	35.395	-14.173	1.00	55.27
	ATOM	664 .	CA	GLY A	120	90.150	35.997	-15.063	1.00	60.24
	MOTA	665	С	GLY A	120	90.723	36.319	-16.427	1.00	63.01
	MOTA	666	. 0	GLY A	120	91.136	35.443	-17.164	1.00	63.92
	MOTA	667	N	GLU A	121	90.729	37.605	-16.750	1.00	64.87
25	ATOM	668	CA	GLU A	121	91.181	38.035	-18.059	1.00	66.91
	ATOM	669	CB	GLU A	121 .	90.002	38.239	-19.003	1.00	67.13
	MOTA	670	CG	GLU A	. 121	.89.872	37.163	-20.053	1.00	67.59
	ATOM	671	CD	GLU A	. 121	88.551	36.456	-19.879	1.00	67.97
	ATOM	672	OE1	GLU A	. 121	88.199	36.107	-18.728	1.00	68.36
30	ATOM	673	OE2	GLU A	121	87.845	36.238	-20.894	1.00	67.22
	MOTA	674	С	GLU A	121	92.000	39.293	-18.102	1.00	68.05
	ATOM	675	0	GLU A	121	91.527	40.416	-18.130	1.00	68.41
	ATOM	676	N	LYS F	122	93.275	38.947	-18.134	1.00	69.16
	ATOM	677	CA	LYS A	A 122	94.495	39.765	-18.380	1.00	70.02
35	MOTA	678	CB	LYS A	122	.94.410	40.220	-19.811	1.00	71.49

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	ATOM	679	CG	LYS	A	122	94.103	39.108	-20.773	1.00	72.69
	MOTA	680	CD	LYS	A	122	94.577	39.506	-22.155	1.00	73.78
	MOTA	68:1	CE	LYS	A	122	94.836	38.285	-23.021	1.00	73.88
	ATOM ·	682	NZ	LYS	A	122	94.892	38.640	-24.471	1.00	74.66
5	ATOM	683	С	LYS	A	122	94.918	40.978	-17.591	1.00	70.09
	MOTA	684	0	LYS	A	122	94.764	42.098	-18.090	1.00	71.62
	MOTA	685	N	LYS	A	123	95.468	40.829	-16.401	1.00	68.95
	MOTA	686	CA	LYS	A	123	95.948	42.044	-15.721	1.00	67.46
	ATOM	687	СВ	LYS	A	123	94.892	43.156	-15.742	1.00	68.33
10	ATOM	688	CG	LYS	A	123	94.578	43.722	-17.135	1.00	69.00
	MOTA	689	CD	LYS	A	123	94.844	45.220	-17.274	1.00	70.0
	ATOM	690	CE	LYS	A	123	94.308	45.768	-18.589	1.00	70.6
	ATOM	691 [.]	ΝZ	LYS	A	123	94.406	47.255	-18.659	1.00	71.09
	MOTA	692	С	LYS	A	123	96.400	41.567	-14.337	1.00	66.42
15	ATOM	693	0	LYS	A	123	96.248	40.376	-14.078	1.00	66.5
	MOTA	694	N	ASP	A	124	96.979	42.356	-13.419	. 1.00	64.9
	ATOM	695	CA	ASP	A	124	97.386	41.763	-12.097	1.00	63.08
	ATOM	696	CB	ASP	A	124	98.581	42.557	-11.470	1.00	64.7
	MOTA	697	CG	ASP	A	124	99.508	41.719	-10.574	1.00	66.6
20	ATOM	698	OD1	ASP	A	124	99.007	40.778	-9.918	1.00	67.3
	ATOM	699	OD2	ASP	A	124	100.713	42.008	-10.527	1.00	67.8
	MOTA	700	C	ASP	A	124	96.195	41.642	-11.147	1.00	60.5
	ATOM	701	0	ASP	A	124	96.279	41.843	-9.928	1.00	60.3
	MOTA	702	N	ĢLU	A	125	95.069	41.253	-11.806	1.00	57.7
25	ATOM	703	CA	GLU	A	125	93.726	41.062	-11.257	1.00	54.5
	MOTA	704	СВ	GLU	A	125	92.680	41.433	-12.338	1.00	54.6
	ATOM	705	CG	GLU	A	125	92.520	40.487	-13.535	1.00	55.4
	ATOM.	706	CD	GLU	A	. 125	91.258	40.811	-14.361	1.00	57.2
	MOTA	707	OE1	GLU	A	. 125	90.365	41.499	-13.828	1.00	57.0
30	MOTA	708	OE2	GLU	A	. 125	91.178	40.368	-15.531	1.00	56.7
	ATOM	709	C	GLU	A	125	93.483	39.673	-10.725	1.00	52.5
	MOTA	710	0	GLU	A	125	93.181	38.746	-11.478	1.00	51.9
	ATOM	711	N.	VAL	, A	126	93.636	39.543	~9.399	1.00	50.1
	MOTA	712	CA	VAL	A	126	93.422	38.271	-8.700	1.00	47.1
					_	126	94.660	37.861	~7.847	3 00	48.5

	ATOM	714	CG1	VAL A 126	95.786	38.882	-7.991	1.00 48.96
	MOTA	715	CG2	VAL A 126	94.272	37.693	-6.385	1.00 49.20
	ATOM	716	С	VAL A 126	92.139	38.282	-7.867	1.00 44.12
	MOTA	717	0	VAL A 126	91.864	39.242 .	-7.137	1.00 44.14
5	ATOM ·	718	N	TYR A 127	91.348	37.221	-8.001	1.00 39.73
	ATOM	719	CA	TYR A 127	90.085	37.115	-7.283	1.00 36.96
	ATOM	720	CB	TYR À 127	88.927	36.904	-8.257	1.00 37.95
	MOTA	721	CG	TYR A 127	88.736	38.015	-9.267	1.00 40.29
	ATOM	722	CD1	TYR A 127	89.358	37.961 -	-10.510	1.00 40.59
10	MOTA	723	CE1	TYR A 127	89.181	38.966 -	-11.439	1.00 42.77
	MOTA	724	CD2	TYR A 127	87.928	39.107	-8.982	1.00 39.85
	ATOM	725	CE2	TYR A 127	87.745	40.119	-9.904	1.00 41.70
	ATOM	726	CZ	TYR A 127	88.374	40.043	-11.133	1.00 42.94
	MOTA	727	ОН	TYR A 127	88.194	41.047	-12.060	1.00 43.28
15	ATOM ·	728.	С	TYR A 127	90.062	35.982	-6.260	1.00 34.06
	MOTA	729	0	TYR A 127	90.468	34.856	-6.543	1.00 33.11
	MOTA	730.	N	LEU A 128	89.502	36.285	-5.089	1.00 31.02
	MOŢA	731	CA	LEU A 128	89.322	35.294	-4.033	1.00 25.83
	ATOM	732	CB	LEU A 128	89.494	35.929	-2.643	1.00 23.26
20	ATOM	733	CG	LEU A 128	88.909	35.128	-1.464	1.00 22.22
	MOTA	734	CD:	1 LEU A 128	89.607	33.777	-1.324	1.00 16.00
	MOTA	735	CD	2 LEU A 128	89.012	35.928	-0.174	1.00 22.36
	MOTA	736	C.	LEU A 128	87.915	34.761	-4.187	1.00 21.88
	ATOM	737	0	LEU A 128	86.983	35.529	-4.414	1.00 23.70
25	ATOM	738	N	ASN A 129	87.755	33.464	-4.112	1.00 20.48
	ATOM	739	ÇA	ASN A 129	86.444	32.869	-4.290	1.00 20.40
	MOTA	740	CB	ASN A 129	86.435		-5.530	1.00 19.61
	MOTA	741	CG	ASN A 129	86.750	32.706	6.826	1.00 18.83
	· ATOM	742	OD	1 ASN A 129	87.882	33.116	-7.070	1.00 18.44
30	ATOM	743	NE	2 ASN A 129	85.738	32.890	-7.649	
	ATOM	744	C	ASN A 129	86.016	32.089	-3.050	
	MOTA	745	0	ASN A 129	86.687	31.155	-2.633	
	MOTA	746	5 N	LEU A 130	84.889	32.481	-2.487	
	ATOM	747	7 C2	A LEU A 130	84.336	31.832		
35	MOTA	748	B CI	B LEU A 130	83.798	32.884	-0.336	1.00 19.16

	MOTA	749	ÇG	LEU Z	A	130	84.842	33.845	0.246	1.00	20.53
	MOTA	750	CD1	LEU 2	A	130	84.192	34.844	1.188	1.00	19.74
	MOTA	751	CD2	LEU .	A	130	85.944	33.083	0.952	1.00	19.17
	MOTA	752	С	LEU ,	A	130	83.212	30.912	-1.720	1.00	18.40
5	MOTA	753	0	LEU .	A	130	82.218	31.364	-2.267	1.00	20,36
	MOTA	754	N	VAL .	A	131	83.366	29.623	-1.453	1.00	17.41
	ATOM	755	CA	VAL .	A	131	82,331	28.658	-1.795	1.00	18.90
	MOTA	756	СВ	VAL .	A	131	82.898	27.362	-2.394	1.00	16.62
	ATOM	757	CG1	VAL .	Ä	131	81.783	26.545	-3.013	1.00	14.67
10	ATOM	758	CG2	VAL .	A	131	83.985	27.672	-3.401	1.00	20.08
•	MOTA	759	С	VAL .	A	131	81.495	28.332	-0.565	1.00	20.30
•	ATOM	760	0	VAL	A	131	81.922	27.587	0.312	1.00	23.54
	MOTA	761	N	LEU	A	132	80.328	28.932	-0.514	1.00	22.83
	ATOM	762	CA	LEU	A	132	79.389	.28.805	0.581	1.00	24.00
15	MOTA	763	СВ	LEU	A	132	78.898	30.211	0.947	1.00	21.47
	MOTA	764	CG	LEU	A	132	79.998	31.233	1.282	1.00	24.67
	MOTA	765	CD1	LEU	A	132	79.629	32.628	0.781	1.00	22.71
	MOTA	766	CD2	LEU	A	132	80.285	31.245	2.784	1.00	20.84
	ATOM	767	С	LEU	A	132	78.189	27.940	0.221	1.00	26.60
20	ATOM	768	0	LEU	A	132	77.920	27.667	-0.956	1.00	26.94
	MOTA	769	N	ASP	A	133	77.448	27.535	1.247	1.00	26.48
	ATOM	770	CA	ASŖ	A	133	76.252	26.732	1.056	1.00	27.70
	MOTA	771	СВ	ASP	A	133	75.722	26.229	2.401	1.00	30.25
	MOTA	772	CG	ASP	A	133	76.219	24.847	2.745	1.00	32.32
25	MOTA	773	OD1	ASP	A	133	76.667	24.644	3.892	1.00	35.29
	ATOM	774	OD2	ASP	A	133	76.163	23.962	1.868	1.00	36.61
	ATOM	.775	С	ASP	A	133	75.197	27.592	0.393	1.00	26.66
	MOTA	776	0	ASP	A	133	75.159	28.798	0.618	1.00	27.07
	ATOM	777	N	TYR	A	134	74.350	26.980	-0.431	1.00	26.84
30	MOTA	778	CA	TYR	A	134	73.311	27.734	-1.127	1.00	25.55
	MOTA	779	CB	TYR	A	134	73.220	27.337	-2.614	1.00	24.53
	MOTA	780	CG	TYR	A	134	72.150	28.097	-3.358	1.00	22.49
	MOTA	781	CD1	TYR	A	134	72.355	29.410	-3.749	1.00	24.18
	MOTA	782	CE1	TYR	A	134	71.368	30.126	-4.404	1.00	26.88
35	ATOM	783	CD2	TYR.	A	134	70.931	27.515	-3.640	1.00	23.64

	ATOM	784	CE2	TYR A	134	69.940	28.218	-4.301	1.00 27.34
	ATOM	785	CZ	TYR A	134	70.166	29.526	-4.678	1.00 25.61
	ATOM	786	ОН	TYR A	134	69.181	30.236	-5.319	1.00 31.37
	ATOM	787	С	TYR A	134	71.950	27.607	-0.453	1.00 23.77
5	ATOM	788	0	TYR A	134	71.436	26.517	-0.286	1.00 26.19
	ATOM	789	N	VAL A	135	71.378	28.747	-0.092	1.00 24.90
	ATOM	790	CA	VAL A	135	70.068	28.829	0 [.] .555	1.00 25.98
	ATOM	791	СВ	VAL A	135	70.231	29.060	2.090	1.00 26.32
	MOTA	7,92	CG1	VAL A	135	68.921	28.837	2.825	1.00 23.53
10	ATOM	793	CG2	VAL A	135	71.303	28.131	2.646	1.00 23.34
	ATOM	794	С	VAL A	135	69.298	29.983	-0.096	1.00 26.48
	MOTA	795	0	VAL A	135	69.67Ô	31.140	0.057	1.00 28.19
	MOTA	796	N	PRO A	136	68.259	29.671	-0.904	1.00 29.01
	ATOM	797	CD	PRO A	136	67.800	28.303	-1.208	1.00 28.45
15	ATOM	798	CA	PRO A	136	67.487	30.682	-1.669	1.00 29.50
	ATOM	799	СВ	PRO P	136	66.720	29.834	-2.687	1.00 29.21 .
	MOTA	800	CG	PRO P	136	66.532	28.532	-1.992	1.00 29.24
	MOTA	801	С	PRO P	A 136	66.516	31.544	-0.869	1.00 27.47
	MOTA	802	0	PRO P	A 136	66.426	32.753	1.095	1.00 27.62
20	MOTA	803	N	GLU A	A 137	65.768	30.946	0.037	1.00 26.71
	ATOM	804	CA	GLU A	A 137	64.814	31.738	0.804	1.00 26.93
	MOTA	805	CB	GLU I	A 137	63.741	30.858	1.440	1.00 28.68
	ATOM	806	CG	GLU	A 137	62.415	30.879		1.00 33.07
	MOTA-	807	CD	GLU	A 137	61.715	32.215		1.00 34.24
25	ATOM	808	OE	l GLU	A 137	62.373	33.253		
	ATOM	809	OE	2 GLU	A 137	60.504	32.225		
	ATOM	810	С	GLU	A 137	65.508			
	MOTA	811	0	GLU	A 137	66.524			
	ATOM	812	N	THR	A 138	64.941			
30	ATOM	813	CA	THR	A 138	65.476			
	ATOM	814	CE	THR	A 138	66.266			
	ATOM	815	00	S1 THR	A 138	65 . 406			
	ATOM	816	C	32 THR	A 138	67.387			
	ATOM	817	C	THR	A 138	64.341			
35	MOTA	818	0	THR	A 138	.63.196	35.24	1 3.489	1.00 19.25

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	ATOM	819	N	VAL A 139	64.66	35.774	5.104	1.00	18.08
	ATOM	820	CA	VAL A 139	63.64	6 36.366	5.963	1.00	15.06
•	ATOM	821	СВ	VAL A 139	64.25	36.775	7.341	1.00	15.44
•	ATOM	822	CG1	VAL A 139	63.26	37.633	8.128	1.00	14.44
5	ATOM	823	CG2	VAL A 139	64.62	28 35.526	8.126	1.00	14.11
	MOTA	824	C	VAL A 139	63.03	37.580	5.273	1.00	13.45
	MOTA	825	0	VAL A 139	61.84	37.840	5.405	1.00	16.40
	MOTA	826	N	TYR A 140	63.85	30.38.304	4.519	1.00	15.51
	ATOM	827	CA	TYR A 140	63.39	39.478	3.777	1.00	18.60
10	ATOM	828	CB	TYR A 140	64.5	72 40.136	3.040	1.00	19.07
	ATOM	829	CG	TYR A 140	64.18	38 41.209	2.042	1.00	22.33
	MOTA	830	CD1	TYR A 140	64.02	26 42.528	2.441	1.00	21.83
	ATOM	831	CE1	TYR A 140	63.6	3 43.515	1.548	1.00	25.48
	MOTA	832	CD2	TYR A 140	63.9	68 40.894	0.696	1.00	24.28
15	ATOM	833	CE2	TYR A 140	63.5	97 41.874	-0.215	1.00	25.55
	MOTA	834	CZ	TYR A 140	63.4	38 43.181	0.213	1.00	28.52
	ATOM	835	ОН	TYR A 140	63.0	70 44.159	-0.687	1.00	29.82
	ATOM	836	C	TYR A 140	62.2	69 39.096	2.802	1.00	19.79
	MOTA	837	0	TYR A 140	61.2	22 39.728	2.778	1.00	21.98
20	MOTA	838	N	ARG A 141	62.4	94 38.046	2.015	1.00	24.14
	MOTA	839	CA	ARG A 141	61.4	98 37.576	1.040	1.00	26.04
	MOTA	840	CB	ARG A 141	62.0	68 36.432	0.193	1.00	29.54
	MOTA	841	CĠ	ARG A 141	62.7	62 36.907	-1.071	1.00	35.28
	MOTA	842	CD	ARG A 141	63.1	84 35.740	-1.960	1.00	40.58
25	MOTA	843	NE.	ARG A 141	63.6	85 36.203	-3.259	1.00	46.87
	MOTA	844	CZ	ARG A 141	64.9	75 36.443	-3.525	1.00	48.90
	MOŢA	845	NH1	ARG A 141	65.9	15 36.179	-2.617	1.00	50.35
	MOTA	846	NH2	ARG A 141	65.3	28 36.940	-4.713	1.00	51.46
	MOTA	847	C	ARG A 141	60.2	20 37.117	1.719	1.00	25.46
30	MOTA	848	. 0	ARG A 141	59.1	.24 37.513	1.330	1.00	25.12
	MOTA	849	N	VAL A 142	60.3	36.278	2.740	1.00	27.17
	ATOM	850	CA	VAL A 142	59.2	209 35.771	3.473	1.00	24.40
	MOTA	851	CB	VAL A 142	59.6	34.807	4.594	. 1.00	24.71
	ATOM	852	CG:	L VAL A 142	58.4	177 34.432	5.487	1.00	24.45
35	ATOM	853	CG:	2 VAL A 142	60.2	295 33.562	3.995	1.00	25.79

	ATOM	854	С	VAL A	112		58.402	36.922	4.059	1 00	23.43		
		855											
	ATOM		0	VAL A	•		57.177	36.899	4.030		26.36		
	ATOM	856		ALA A				37.927	4.584		23.47		
5	ATOM	857		ALA A			58.492	39.111	•		22.83		
3	ATOM	858		ALA A			59.569	39.970	5.858		20.91		
	ATOM	859	C .	ALA A			57.693	39.918	4.176		20.62		
	ATOM	860		ALA A	,		56.521	40.225	4.384	1.00	17.83		
	ATOM	.861	N	ARG A	144		58.325	40.237	3.052	1.00	24.31		
_	MOTA	862	CA	ARG A	144		57.650	40.983	1.977	1.00	23.67		
10	MOTA	863	CB	ARG A	144		58.635	41.269	0.844	1.00	26.35		
	ATOM	864	CG	·ARG A	144		58.023	42.018	-0.327	1.00	29.59		
•	MOTA	.865	CD	ARG A	144 .		59.045	42.234	-1.425	1.00	29.52		
	ATOM	866	NE	ARG. A	144		59.470	40.973	-2.016	1.00	32.38		
	ATOM	867	CZ	ARG A	144		60.603	40.819	-2.699	1.00	33.78		
15	ATOM	868	NHl	ARG A	144		61.368	41.874	-2.977	1.00	34.65		
	MOTA	869	NH2	ARG A	144		60.962	39.609	-3.123	1.00	34.37	•	
	MOTA	870	С	ARG A	144		56.453	40.190	1.469	1.00	22.19		
	ATOM	871	0	ARG A	144		55.399	40.749	1.181	1.00	23.86		
	ATOM	872	N	HIS A	145		56.611	38.876	1.413	1.00	23.70		
20	ATOM	873	CA	HIS A	145	•	55.545	37.970	0.988	1.00	26.97		
	MOTA	874	СВ	HIS A	145		56.062	36.525	1.009	1.00	30.84		
	ATOM	875	CG	HIS A	145		55.056	35.464	0.707	1.00	36.75	•	
	ATOM	876	CD2	HIS A	145		54.720	34.344	1.401	11.00	38.92		
	ATOM	877	ND1	HIS A	145		54.269	35.458	-0.435	1.00	39.38		
25	MOTA	878	CE1	HIS A	145		53.495	34.383	-0.429	1.00	40.00		
	ATOM	879	NE2	HIS A	145		53.751	33.691	0.677	1.00	41.00		
	MOTA	880	С	HIS A	145		54.290	38.159	1.852	1.00	27.08		
	ATOM	881	0	HIS A	145		53.188	38.312	1.320	1.00	26.89		
	ATOM	882	N	TYR A	146		54.463	38.203	3.194	1.00	26.20		
30	MOTA	883	CA	TYR A	146		53.329	38.432	4.116	1.00	23.27		
	MOTA	884	СВ	TYR A	146		53.707	38.079	5.566	1.00	21.78		
	ATOM	885	CG	TYR A	146		53.640	36.608	5.837	1.00	16.94		
	MOTA	886	CD1	TYR A	146		54.716	35.793	5.563	1.00	15.65		
	ATOM	887	CE1	TYR A	146		54.641	34.434	5.758	1.00	15.99	-	
35	MOTA	888	CD2	TÝR A	146		52.484	36.034	6.314	1.00	15.27		
												•	

	ATOM	889	CE2	TYR A	146	52.408	34.673	6.520	1.00	16.80
	ATOM	890	CZ	TYR A	146 .	53.485	33.884	6.238	1.00	14.45
	MOTA	891	ОН	TYR A	146	53.403	32.526	6.431	1.00	18.28
	MOTA	892	C	TYR A	146	52.867	39.879 .	4.044	1.00	22.91
5	MOTA	893	0	TYR A	146	51.681	40.168	4.096	1.00	22.73
	MOTA	894	N	SER A	147	53.827	40.780	3.913	1.00	25.91
	MOTA	895	CA	SER A	147	53.567	42.218	3.816	1.00	29.26
	ATOM	896	CB	SER A	147	54.904	42.962	3.732	1.00	29.44
•	ATOM	897	OG	SER A	147	54.724	44.295	3.311	1.00	34.56
10	ATOM .	898	C	SER A	147	52.667	42.571	2.606	1.00	31.47
	MOTA	899	0	SER A	147	51.723	43.361	2.733	1.00	30.92
	MOTA	900	N	ARG A	148	52.959	41.979	1.436	1.00	32.82
	MOTA	901	CA	ARG A	148	52.172	42.240	0.221	1.00	34.38
	ATOM	902	CB	ARG A	148	52.801	41.544	-0.979	1.00	35.40
15	ATOM	903	CG	ARG A	148	53.649	42.476	-1.818	1.00	35.95
	ATOM	904	CD	ARG A	148	54.822	41.747	-2.445	1.00	37.90
	ATOM	905	NE	ARG A	148	55.806	42.672	-2.977	1.00	38.82
	ATOM	906	CZ	ARG A	148	56.864	42.291	-3.674	1.00	41.01
	ATOM	907	NH1	ARG A	148	57.058	41.002	-3.949	1.00	41.88
20	MOTA	908	NH2	ARG A	148	57.734	43.200	-4.101	1.00	41.62
	ATOM	909	C	ARG A	148	50.714	41.802	0.385	1.00	34.50
	MOTA	910	0	ARG A	148	49.798	42.417	-0.173	1.00	35.04
	ATOM	911	N	ALA A	149 ·	50.492	40.766	1.179	1.00	33.08
	ATOM	912	CA	ALA A	149	49.136	40.306	1.429	1.00	32.56
25	ATOM	913	CB	ALA A	149	49.116	38.800	1.624	1.00	32.41
	MOTA	914	С	ALA A	149	48.535	41.021	2.647	1.00	32.79
	ATOM	915	0	ALA A	149	47.471	40.639	3.124	1.00	33.04
	ATOM	916	N	LYS A	150	49.233	42.054	3.155	1.00	34.10
	ATOM	917	CA	LYS A	150	48.776	42.804	4.328	1.00	34.50
30	MOTA	918	CB	LYS A	150	47.474	43.560	4.023	1.00	34.90
	ATOM	919	CG	LYS A	150	47.633	44.680	3.001	1.00	36.28
	MOTA	920	CD	LYS A	. 150	48.720	45.668	3.405	1.00	38.33
	ATOM	921	CE .	LYS A	150	48.615	46.983	2.636	1.00	40.38
	ATOM	922	NZ	LYS A	150	49.673	47.109	1.583	1.00	41.77
35	ATOM	923	С	LYS A	150	48.589	41.851	5.508	1.00	34.57

	MOTA	924	0	LYS A	150	47.651	41.981	6.293	1.00 34.54
	ATOM	925	N	GLN A	151	49.483	40.872	5.599	1.00 34.09
	ATOM	926	CA	GLN A	151	49.417	39.868	6.645	1.00 34.74
	ATOM	927	CB	GLN A	151	49.142	38.500	6.043	1.00 35.68
5	ATOM	928	CG	GLN A	151	47.699	38.313	5.622	1.00 38.01
	MOTA	929	CD	GLN A	151	47.309	36.860	5.577	1.00 38.94
	ATOM	930	OE1	GLN A	151	48.170	35.982	5.527	1.00 37.93
	ATOM	931	NE2	GLN A	151	46.004	36.596	5.599	1.00 39.52
	ATOM	932	C	GLN A	151	50.669	39.818	7.501	1.00 34.35
10	ATOM	933	0	GLN A	151	51.739	40.266	7.100	1.00 32.05
	ATOM	934	Ņ	THR A	152	50.506	39.263	8.698	1.00 34.62
	MOTA	935	CA	THR A	152	51.588	39.132	9.661	1.00 34.27
	MOTA	936	СВ	THR A	152	51.033	39.416	11.078	1.00 36.00
	MOTA	937	OG1	THR A	152	50.127	40.515	11.083	1.00 37.75
15	MOTA	938	CG2	THR A	152	52.091	39.668	12.129	1.00 35.72
	ATOM	939	С	THR A	. 152	52.160	37.723	9.623	1.00 31.15
	MOTA	940	0	THR A	152	51.415	36.759	9,512	1.00 32.52
	ATOM	941	N	LEU A	. 153	53.471	37.604	9.766	1.00 30.45
	MOTA	942	CA	LEU A	. 153	54.108	36.292	9.808	1.00 30.39
20	ATOM	943	CB	LEU A	. 153	55.623	36.452	9.713	1.00 32.03
	MOTA	944	CG	LEU A	. 153	56.444	35.160	9.724	1.00 32.38
•	MOTA	945	CD1	LEU A	. 153	56.138	34.318	8.494	1.00 33.99
	MOTA	946	CD2	LEU A	153	57.931.	35.469	9.808	1.00 33.12
·	MOTA	947	С	LEU A	153	53.752	35.619	11.145	1.00 29.43
25	MOTA	948	0	LEU P	153	53.857	36.243	12.195	1.00 28.63
	ATOM	949	N	PRO .F	154	53.280	34.356	11.133	1.00 28.74
·	MOTA	950	CD	PRO F	A 154	53.046	33.527	9.930	1.00 27.55
	ATOM	951	CA	PRO P		52.888	33.651	12.369	1.00 27.14
20	ATOM	952	CB		154	52.653		11.895	1.00 27.21
30	ATOM ,	953	CG ·		A 154	52.190	32.414	10.479	1.00 30.24
	MOTA	954	С		A 154.	53.966	33.717	13.452	1.00 23.50
	MOTA	955	0		A 154	55.105	33.353	13.218	1.00 24.23
	ATOM	956	N		A 155	53.579	34.204	14.634	1.00 22.72
2.5	ATOM	957			A 155	54.476	34.360	15.800	1.00 20.53
35	ATOM	958	′ CB	VAL	A 155	53.685	34.678	17.102	1.00 23.34
		•					•		

	ATOM	959	CG1	VAL A	155·	54.507	34.387	18.361	1.00	24.21
	MOTA	960	CG2	VAL A	155	53.226	36.124	17.092	1.00	20.95
	MOTA	961	С	VAL A	155	55.414	33.177	16.007	1.00	16.62
	ATOM	962	0	VAL A	155	56.576	33.366	16.328	1.00	20.84
5	ATOM	963	N	ILE A	156	54.933	31.960	15.807	1.00	18.03
	ATOM	964	CA	ILE A	156	55.790	30.790	15.965	1.00	19.48
	ATOM	965	CB	ILE A	156	55.043	29.441	15.759	1.00	21.25
	ATOM	966	CG2	ILE A	156	54.460	29.328	14.356	1.00	23.81
	ATOM	967	CG1	ILE A	156	55.971	28.257	16.041	1.00	21.62
10	ATOM	968	CD1	ILE A	156	56.329	28.079	17.507	1.00	23.55
	ATOM	969.	С	ILE A	156	57.032	30.878	15.064	1.00	21.28
•	ATOM	970	0	ILE A	156	58.115	30.419	15.450	1.00	23.11
	ATOM	971	N	TYR A	157	56.875	31.498	13.869	1.00	21.30
	MOTA	972	CA	TYR A	157	57.993	31.669	12.920	1.00	20.67
15	ATOM	973	CB	TYR A	157	57.466	31.982	11.503	1.00	22.40
	MOTA	974	CG	TYR A	157	56.837	30.800	10.804	1.00	20.61
	MOTA	975	CD1	TYR A	157	55.507	30.824	10.439	1.00	23.85
	MOTA	976	CE1	TYR A	157	54.922	29.748	9.808	1.00	26.60
	MOTA	977	CD2	TYR A	157	57.578	29.665	10.519	1.00	22.96
20	MOTA	978	CE2	TYR A	157	57.003	28.581	9.889	1.00	26.14
	MOTA	979	CZ	TYR A	157 .	55.673	28.631	9.536	1.00	27.11
	ATOM	980	ОН	TYR A	157	55.092	27.558	8.905	1.00	32.33
	MOTA	981	С,	TYR A	157	58.907	32.791	13.388	1.00	17.50
	ATOM.	982	0	TYR A	157	60.119	32.722	13.270	1.00	16.80
25	ATOM	983	И	VAL A	158	58.317	33.824	13.939	1.00	17.44
	ATOM	984	CA	VAL A	158	59.108	34.928	14.442	1.00	18.24
	MOTA	985	CB	VAL A	158	58.214	36.067	14.939	1.00	20.43
	MOTA	986	CG1	VAL A	158	59.055	37.177	15.559	1.00	19.36
	MOTA	987	CG2	VAL A	158	57.359	36.605	13.801	1.00	18.19
30	MOTA	988	С	VAL A	158	60.014	34.432	15.574	1.00	17.07
	ATOM	989	0	VAL A	. 158	61.174	34.805	15.658	1.00	18.46
	MOTA	990	N	LYS A	159	59.480	33.560	16.428	1.00	18.82
	ATOM	991	CA	LYS A	159	60.264	33.002	17.545	1.00	19.42
	ATOM	992	CB	LYS A	. 159	59.362	32.146	18.441	1.00	16.16
35	ATOM	993	CG	LYS A	159	58.585	32.971	19.446	1.00	18.16

	ATOM	994	CD	LYS A 159	57.569	32.135	20.217	1.00	19.52
	MOTA	995	CE	LYS A 159	56.559	33.019	20.938	1.00	20.28
	MOTA	996	NZ	LYS A 159	55.522	32.220	21.646	1.00	22.23
	ATOM	997	С	LYS A 159	61.434	32.179	17:050	1.00	18.62
5	MOTA	998	0.	LYS A 159	62.589	32.436	17.411	1.00	18.36
	MOTA	999	N	LEU A 160	61.121	31:178	16.225	1.00	20.14
	MOTA	1000	CA	LEU A 160	62.120	30.274	15.661	1.00	19.50
	ATOM	1001	CB	LEU A 160	61.466	29.267	14.706	1.00	19.84
	MOTA	1002	CG	LEU A 160	60.808	28.051	15.365	1.00	22.33
10	ATOM	1003	CD1	LEU A 160	59.638	27.550	14.528	1.00	22.99
	ATOM	1004	CD2	LEU A 160	61.828	26.945	15.596	1.00	22.73
	ATOM	1005	С	LEU A 160	63.224	31.012	14.948	1.00	18.91
	MOTA	1006	0	LEU A 160	64.397	30.708	15.142	1.00	19.83
	MOTA	1007	N	TYR A 161	62.860	31.967	14.113	1.00	17.95
15	ATOM	1008	CA	TYR A 161	63.865	32.719	13.366	1.00	20.81
	MOTA	1009	CB	TYR A 161	63.218	33.585	12.257	1.00	21.26
	· MOTA	1010	CG	TYR A 161	62.470	32.792	11.198	1.00	23.48
	MOTA	1011	CD1	TYR A 161	62.769	31.463	10.954	1.00	23.93
	MOTA	1012	CE1	TYR A 161	62.064	30.738	10.009	1.00	29.23
20	MOTA	1013	CD2	TYR A 161	61.450	33.376	10.466	1.00	24.92
	MOTA	1014	CE2	TYR A 161	60.744	32.665	9.516	1.00	27.72
	MOTA	1015	CZ	TYR A 161	61.051	31.348	9.291	1.00	28.92
	MOTA	1016	ОН	TYR A 161	60.343	30.631	8.348	1.00	32.19
•	MOTA	1017	C	TYR A 161	64.725	33.592	14.267	1.00	19.07
25	MOTA	1018	0	TYR A 161	65.943	33.579	14:159	1.00	20.35
	MOTA	1019	Ŋ	MET A.162	64.078	34.382	15.130	1.00	19.27
	MOTA .	1020	CA	MET A 162	64.808	35.296	16.026	1.00	17.97
	MOTA	1021	СВ	MET A 162	63.843	36.243	16.743	1.00	18.49
	MOTA	1022	CG	MET A 162	63.234	37.287	15.810	1.00	20.41
30	MOTA	1023	SD	MET A 162	64.483	38.213	14.898	1.00	22.51
	MOTA	1024	CE	MET A 162	65.609	38.696	16.222	1.00	21.98
	MOTA	1025	С	MET A 162	65.717	34.556	16.997	1.00	14.30
	MOTA	1026	0	MET A 162	66.844	34.977	17.247	1.00	18.15
	ATOM	1027	N	TYR A 163	65.250	33.433	17.508	1.00	15.87
35	MOTA	1028	CA	TYR A 163	66.055	32.616	18.431	1.00	17.26

	ATOM	1029	СВ	TYR	A	163		.65.225	31.385	18.868	1.00	16.49
	ATOM	1030	CG	TYR	A	163		65.952	30.442	19.801	1.00	17.42
	ATOM	1031	CD1	TYR	A	163		65.926	30.620	21.194	1.00	18.67
	ATOM	1032	CE1	TYR	A	163		66.623	29.762	22.037	1.00	16.89
5	ATOM	1033	CD2	TYR	A	163		66.684	29.381	19.291	1.00	16.80
	ATOM	1034	CE2	TYR	A	163		67.371	28.525	20.111	1.00	18.00
	MOTA	1035	CZ	TYR	A	163		67.341	28.722	21.492	1.00	20.67
	ATOM	1036	OH	TYR	A	163		68.062	27.886	22.302	1.00	20.49
	MOTA	1037	С	TYR	A	163		67.367	32.182	17.770	1.00	18.07
10	ATOM	1038	0	TYR	A	163		68.480	32.385	18.309	1.00	20.01
	ATOM	1039	N	GLN	A	164	÷	67.244	31.585	16.579	1.00	17.19
	ATOM	1040	CA	GLN	A	164	•	68.410	31.118	15.826	1.00	12.78
	MOTA	1041	CB	GLN	A	164		67.966	30.351	14.569	1.00	14.61
	MOTA	1042	CG	GLN	A	164		67.389	28.990	14.899	1.00	14.23
15	MOTA	1043	CD	GLN	A	164		66.632	28.353	13.751	1.00	16.46
	ATOM	1044	OE1	GLN	A	164		65.450	28.584	13.578	1.00	17.33
	MOTA	1045	NE2	GLN	A	164		67.312	27.522	12.981	1.00	12.47
	MOTA	1.046	С	GLN	P	164		69.396	32.233	15.520	1.00	8.49
	MOTA	1047	0	GLN	P	164		70.590	32.015	15.536	1.00	9.26
20	ATOM	1048	N	LEU	P	165		68.883	33.437	15.282	1.00	11.16
	ATOM	1049	CA	LEU	I	A 165		69.712	34.619	15.011	1.00	11.15
	MOTA	1050	CB	LEU	J P	A 165		68.797	35.799	14.635	1.00	9.98
	MOTA	1051	CG	LEÙ	J A	165		69.420	36.939	13.825	1.00	
	ATOM	1052	CDI	LEC	J Z	A 165		68.899	38.285	14.272	1.00	13.53
25	MOTA	1053	CD2	. LET	J Z	A 165		70.930	36.916	13.817	1.00	14.22
	ATOM	1054	С	LE	ן ז	A 165		70.499	35.006	16.266	1.00	10.07
	ATOM	1055	0	LE	נ נ	A 165		71.696	35.258	16.226	1.00	11.99
	ATOM	1056	N	PH!	Ē.	A 166	•	69:806	35.058	17.391	1.00	12.97
	ATOM	1057	CA	PH!	E ,	A 166		70.474	35.408	18.652	1.00	13.16
30	MOTA	1058	СВ	PH	E	A 166		69.441	35.524	19.778	1.00	9.30
	ATOM	1059	CG	PH	E	A 166		68.706	36.825	19.704	1.0	5.00
	ATOM	1060	CD	1 PH	E	A 166		67.345	36.861	19.600	1.0	0 5.00
	ATOM	1061	. CD	2 PH	E	A 166		69.396	38.007	19.743	1.0	0 5:00
	ATOM	1062	CE	l PH	E	A 166		66.673	38.054	19.544	1.0	0 5.00
35	MOTA	1063	CE	2 PH	E	A 166		68.733	39.208	19.682	1.0	0 7.78

		ATOM	1064	CZ	PHE A	166	67.370	39.228	19.586	1.00	6.07
		ATOM	1065	C .	PHE A	166	71.557	34.396	18.943	1.00	9.24
		MOTA	1066	0	PHE A	166	72.679	34.743	19.273	1.00	14.23
		ATOM	1067	N	ARG A	167	71.238	33.147	18.736	1.00	11.80
	5	MOTA	1068	CA	ARG A	167	72.210	32.087	18.915	1.00	14.27
		ATOM .	1069	CB	ARG A	167	71.542	30.754	18.618	1.00	17.59
		ATOM	1070	CG	ARG A	167	71.692	29.753	19.734	1.00	20.33
		MOTA	1071	CD	ARG A	167	72.416	28.515	19.268	1.00	19.92
		MOTA	1072	NE	ARG A	167	71.499	27.404	19.111	1.00	20.11
	10	ATOM	1073	CZ	ARG A	167	71.873	26.132	19.040	1.00	19.61
		MOTA	1074	NH1	ARG A	167	73.150	25.796	19.095	1.00	20.92
•		ATOM	1075	NH2	ARG A	167	70.950	25.191	18.916	1.00	23.68
		ATOM	1076	C ·	ARG A	167	73.439	32.284	18.020	1.00	18.46
		MOTA	1077	0	ARG A	167	74.591	32.262	18.498	1.00	19.88
	15	ATOM	1078	И	SER A	168	73.224	32.492	16.707	1.00	18.03
		ATOM	1079	CA	SER A	168	74.380	32.704	15.820	1.00	16.37
		ATOM	1080	СВ	SER A	168	73.950	32.854	14.337	1.00	13.75
	•	ATOM	1081	OG	SER A	168	73.376	34.123	14.092	1.00	10.05
		ATOM	1082	C	SER A	168	75.171	33.928	16.291	1.00	14.44
	20	MOTA	1083	0	SER A	168	76.397	33.940	16.249	1.00	15.57
		MOTA	1084	N	LEU A	169	74.460	34.952	16.763	1.00	13.04
		MOTA	1085	CA	LEU A	169	75.127	36.170	17.264	1.00	15.39
		MOTA	1086	CB.	LEU A	169 [.]	74.098	37.253	17.578	1.00	15.44
		MOTA	1087	CG	LEU A	169 .	73.461	37.955	16.369	1.00	17.31
	25	MOTA	1088	CD1	LEU A	169	72.451	38.999	16.826	1.00	12.89
		MOTA	1089	CD2	LEU A	169	74.535	38.608	15.514	1.00	12.28
	•	MOTA	1090	С	LEU A	169	75.979	35.855	18.511	1.00	14.46
		MOTA	1091	0	LEU A	169	77.130	36.263	18.611	1.00	14.94
		MOTA	1092	И.	ALA A	170	75.413	35.083	19.438	1.00	17.16
	30	MOTA	1093	CA	ALA A	170	76.135	34.678	20.653	1.00	18.82
		MOTA	1094	CB	ALA A	170	75.251.	33.764	21.513	1.00	18.42
		MOTA	1095	C ·	ALA A	170	77.425	33.964	20.279	1.00	18.95
		ATOM	1096	0	ALA A	170	78.518	34.272	20.800	1.00	19.35
		ATOM .	1097	N	TYR A	171	77.303	33.011	19.358	1.00	19.08
	35	ATOM	1098	CA	TYR A	171	78.455	32.251	18.897	1.00	16.90

•	ATOM	1099	CB	TYR A	171	78.033	31.178	17.884	1.00	17.64
	MOTA	1100	CG	TYR A	171	79.187	30.407	17.276	1.00	17.25
	MOTA	1101	CD1	TYR A	171	79.791	29.354	17.957	1.00	15.43
	MOTA	1102	CE1	TYR A	171	80.836	28.648	17.394	1.00	17.19
5	MOTA	1103	CD2	TYR A	171	79.667	30.735	16.013	1.00	15.34
	ATOM	1104	CE2	TYR A	171	80.717	30.035	15.439	1.00	15.84
	MOTA	1105	CZ	TYR A	171	81.294	28.998	16.125	1.00	18.87
	MOTA	1106	ОН	TYR A	171	82.328	28.299	15.551	1.00	20.53
	MOTA	1107	С	TYR A	171	79.551	33.149	18.345	1.00	16.46
10	ATOM	1108	0	TYR A	171	80.717	33.012	18.719	1.00	18.03
	MOTA	1109	N	ILE A	172	79.203	34.073	17.449	1.00	16.80
	ATOM	1110	CA	ILE A	172	80.235	34.947	16.878	1.00.	16.95
	ATOM	1111	CB	ILE A	172	79.798	35.670	15.572	1.00	15.99
	ATOM	1112	CG2	ILE A	172	79.655	34.672	14.435	1.00	18.73
15	MOTA	1113	CG1	ILE A	172	78.488	36.437	15.769	1.00	16.30
	ATOM	1114	CD1	ILE A	172	78.254	37.509	14.728	1.00	18.08
	MOTA	1115	С	ILE A	172	80.744	35.949	17.892	. 1.00	15.06
	MOTA	1116	0	ILE A	172	81.937	36.187	17.987	1.00	14.81
	MOTA	1117	N	HIS A	173	79.834	36.527	18.662	1.00	16.56
20	MOTA	1118	CA	HIS A	173	80.230	37.494	19.692	1.00	17.03
	MOTA	1119	CB	HIS A	173	78.991	38.097	20.377	1.00	16.14
	MOTA	1120	CG	HIS A	. 173	78.208	39.002	19.467	1.00	14.02
	MOTA	1121	CD2	HIS A	. 173	78.483	39.454	18.197	1.00	13.45
	MOTA	1122	ND1	HIS A	. 173	77.015	39.594	19.825	1.00	12.19
25	ATOM	1123	CE1	HIS A	173	76.587	40.372	18.826	1.00	14.81
	MOTA	1124	NE2	HIS A	173	77.466	40.300	17.831	1.00	10.44
	MOTA	1125	C	HIS. A	173	81.225	36.849	20.687	1.00	17.24
	ATOM	1126	0	HIS A	173	82.097	37.540	21.205	1.00	20.12
	ATOM	1127	N	SER A	174	81.130	35.508	20.877	1.00	17.18
30	ATOM	1128	CA	SER P	174	82.043	34.715	21.747	1.00	18.95
	MOTA	1129	CB	SER A	174	81.725	33.214	21.672		18.66
	ATOM	1130	OG	SER A	174	80.376	32.963	21.936	1.00	29.03
	ATOM	1131	. C	SER A	174	83.499	34.857	21.344	1.00	20.81
	ATOM	1132	0	SER A	A 174	84.400	34.758	22.196	1.00	18.20
35	MOTA	1133	N	PHE A	A 175	83.732	35.042	20.035	1.00	18.33

	ATOM	1134	CA	PHE A	175	85.079	35.164	19.488	1.00	18.92
	ATOM	1135	CB	PHE A	175	85.156	34.469	18.111	1.00	20.09
	ATOM	1136	CG	PHE A	175	85.081	32.969	18.177	1.00	18.05
	MOTA	1137	CD1	PHE A	175	86.215	32.221 .	18.380	1.00	18.98
5	MOTA	1138	CD2	PHE A	175	83.875	32.317	18.051	1.00	19.83
	ATOM	1139 ·	CE1	PHE- A	175	86.151	30.849	18.455	1.00	19.35
	MOTA	1140	CE2	PHE A	175	83.804	30.945	18.124	1.00	19.15
	ATOM	1141	CZ	PHE A	175	84.943	30.211	18.327	1.00	17.42
	ATOM	1142	С	PHE A	175	85.484	36.615	19.330	1.00	18.22
10	ATOM	1143	0	PHE A	175	86.571	36.903	18.831	1.00	21.16
	MOTA	1144	N	GLY A	176	84.599	37.528	19.727	1.00	18.25
•	MOTA	1145	CA	GLY A	176	84.878	38.955	19.591	1.00	18.73
	ATOM	1146	С	GLY A	176	84.541	39.492	18.193	1.00	18.75
	ATOM	1147	0	GLY A	176	84.909	40.614	17.844	1.00	16.75
15	ATOM	1148	N	ILE A	177	83.844	38.675	17.400	1.00	18.95
	MOTA	1149	CA .	ILE A	177	83.459	39.023	16.023	1.00	17.03
	ATOM	1150	CB	ILE A	177	83.391	37.750	15.144	1.00	18.98
	ATOM	1151 -	CG2	ILE A	177	82.803.	38.078	13.767	1.00	20.31
	ATOM	1152	CG1	ILE A	177	84.770	37.106	15.031	1.00	16.05
20	ATOM	1153	CD1	ILE A	177	84.720	35.603	14.862	1.00	17.66
	MOTA	1154	С	ILE A	177	82.107	39.713	15.933	1.00	13.93
•	MOTA	1155	0	ILE A	177	81.087	39.148	16.280	1.00	16.03
	MOTA	1156	N	CYS A	178	82.107	40.917	15.407	1.00	12.55
	MOTA	1157	CA	CYS A	178	80.887	41.662	15.204	1.00	13.12
25	ATOM	1158	CB	CYS A	. 178	81.095	43.115	15.644	1.00	12.26
	ATOM	1159	SG	CYS A	. 178	79.577	44.043	15.818	1.00	21.65
	MOTA	1160	С	CYS A	. 178	80.521	41.604	13.699	1.00	15.33
	ATOM	1161	0	CYS A	. 178	81.362	41.910	12.845	1.00	17.46
	ATOM	1162	N	HIS A	. 179	79.294	41.183	13.409	1.00	14.88
30	ATOM	1163	CA	HIS A	. 179	78.779	41.037	12.050	1.00	18.49
	MOTA	1164	CB	HIS P	179	77.380	40.418	12.066	1.00	16.51
	MOTA	1165	CG	HIS F	179	76.978	39.835	10.736	1.00	19.21
	ATOM	1166	CD2	HIS A	179	77.365	38.698	10.109	1.00	18.67
	MOTA	1167	ND1	HIS F	A 179	76.083	40.442	9.882	1.00	16.97
35	ATOM	1168	CE1	HIS A	A 179	75.938	39.711	8.799	1.00	13.99

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	MOTA	1169	NE2	HIS A	Ą	179		76.705	38.649	8.912	1.00	15.08
	MOTA	1170	C	HIS A	A	179		78.767	42.383	11.325	1.00	20.60
	MOTA	1171	0	HIS I	A	179		79.474	42.552	10.338	1.00	17.90
	ATOM	1172	N	ARG Z	A	180		77.980	43.331	11.875	1.00	19.78
5	ATOM	1173	CA	ARG A	A	180		77.862	44.697	11.369	1.00	19.72
	ATOM	1174	CB	ARG A	A	180		79.237	45.298	11.122	1.00	22.50
	MOTA	1175	CG	ARG	A	180		80.046	45.492	12.395	1.00	20.08
	ATOM	1176	·CD	ARG .	A.	180		81.157	46.504	12.195	1.00	20.28
	ATOM	1177	NE	ARG .	A	180		82.159	46.023	11.247	1.00	22.10
10	MOTA	1178	CZ	ARG .	A	180	•	83.174	46.749	10.797	1.00	19.60
	ATOM	1179	NH1	ARG .	A	180	-	83.369	47.979	11.242	1.00	20.78
	MOTA	1180	NH2	ARG .	A	180		84.005	46.229	9.907	1.00	20.16
. •	ATOM	1181	С	ARG	A	180		76.971	44.837	10.121 :	1.00	19.93
	MOTA	1182	0	ARG	A	180		76.937	45.907	9.506	.1.00	18.32
15	ATOM	1183	N	ASP	A	181		76.218	43.793	9.784	1.00	20.47
	ATOM	1184	CA	ASP	A	181		75.305	43.846	8.640	1.00	22.91
	MOTA	1185	CB	ASP	A	181		76.048	43.534	7.319	1.00	20.92
	MOTA	1186	CG	ASP	A	181		75.296	43.997	6.056	1.00	24.19
	ATOM	1187	OD1	ASP	Ą	181		74.353	44.814	6.170	1.00	20.69
20	MOTA	1188	OD2	ASP	A	181		75.663	43.529	4.948	1.00	22.69
	MOTA	1189	С	ASP	A	181		74.106	42.930	8.853	1.00	22.26
	ATOM	1190	0	ASP	A	181		73.738	42.132	7.980	1.00	22.03
	MOTA	1191	N	ILE	A	182		73.486	43.061	10.041	1.00	21.81
	ATOM	1192	CA	ILE	A	182		72.330	42.277	10.419	1.00	17.10
25	ATOM	1193	CB	ILE	A	182		72.215	42.135	11.959	1.00	18.31
	MOTA	1194	CG2	ILE	A	182		70.918	41.438	12.353	1.00	15.65
	ATOM	1195	CG1	ILE	A	182		73.431	41.377	12.489	1.00	16.67
	MOTA	1196	CD1	ILE	A	182		73.369	39.879	12.244	1.00	15.69
	MOTA	1197	C .	ILE	A	182		71.056	42.859	9.841	1.00	17.49
30	ATOM	1198	0	ILE	A	182		70.618	43.954	10.222	1.00	17.73
	MOTA	1199	N	LYS	A	183		70.482	42.115	8.903	1.00	14.95
	ATOM	1200	CA	LYS	A	183		69.273	42.519	8.220	1.00	12.48
	MOTA	1201	CB	LYS	A	183		69.614	43.479	7.071	1.00	17.35
	ATOM	1202	CG	LYS	A	183		70.456	42.850	5.959	1.00	14.20
35	MOTA	1203	CD	LYS	A	183		71.084	43.921	5.087	1.00	17.19

	MOTA	1204	CE	LYS A	A	183	71.955	43.310	4.001	1.00	20.09
	MOTA	1205	NZ	LYS :	A	183	72.604	44.349	3.158	1.00	17.13
	MOTA	1206	С	LYS :	A	183	68.548	41.288	7.705	1.00	8.04
	ATOM	1207	0	LYS .	A	183	69.132	40.220	7.644	1.00	8.53
5	MOTA	1208	N	PRO .	A	184	67.270	41.414	7.360	1.00	7.13
	MOTA	1209	CD	PRO .	A	184	66.505	42.647	7.427	1.00	6.34
	ATOM	1210	CA	PRO .	A	184	66.460	40.292	6.884	1.00	11.96
	ATOM	1211	CB	PRO .	A	184	65.121	40.928	6.544	1.00	10.86
	ATOM	1212	CG	PRO	A	184	65.096	42.183 .	7.334	1.00	8.34
10	ATOM	1213	C	PRO	A	184	67.030	39.540	5.668	1.00	14.64
	ATOM	1214	0	PRO	A	184	66.792	38.343	5.527	1.00	18.32
-	MOTA	1215	N	GLN	A	185	67.771	40.226	4.788	1.00	17.59
	MOTA	1216	CA	GLN	A	185	68.319	39.545	3.610	1.00	19.45
	MOTA	1217	CB	GLN	A _.	185	68.582	40.495	2.431	1.00	22.98
15	MOTA	1218	CG	GLN	A	185	69.181	41.826	2.809	1.00	28.27
	MOTA	1219	CD	GLN	A	185	68.121	42.897	2.974	1.00	32.07
•	MOTA	1220	OE1	GLN	A	185	67.725	43.533	1.993	1.00	32.64
	MOTA	1221	NE2	GLN	A	185	67.657	43.105	4.223	1.00	26.42
	MOTA	1222	С	GLN	A	185	69.544	38.734	3.938.	1.00	19.77
20	MOTA	1223	0	GLN	A	185	69.951	37.860	3.150	1.00	16.26
	ATOM .	1224	N	ASN	A	186	70.135	38.997	5.117	1.00	17.25
	ATOM	1225	CA	ASN	A	186	71.311	38.244	5.532	1.00	15:26
	ATOM	1226	CB	ASN	A	186	72.408	39.145	6.120	1.00	17.32
	ATOM	1227	CG	ASN	-A	186	73.194	39.859	5.019	1.00	19.75
25	ATOM	1228	ODÍ	ASN	A	186	73.140	39.464	3.844	1.00	19.21
	ATOM	1229	ND2	ASN	A	186	73.931	40.899	5.376	1.00	16.18
	MOTA	1230	C	ASN	A	186	70:942	37.030	6.401	1.00	13.78
	ATOM	1231	0	ASN	A	186	71.800	36.359	6.966	1.00	14.79
•	ATOM	1232	N	LEU	A	187	69.658	36.745	6.447	1.00	14.07
30	ATOM	1233	CA	LEU	A	187	69.098	35.618	7.182	1.00	16.11
	ATOM	1234	CB	LEU	A	187	68.023	36.114	8.160	1.00	13.53
•	ATOM	1235	CG	LEU	A	187	68.465	37.246	9.086	1.00	14.77
	MOTA	1236	CD1	LEU	A	187	67.284	37.829	9.849	1.00	12.78
	MOTA	1237	CD2	. ren	A	187	69.573	36.763	10.004	1.00	14.06
35	MOTA	1238	С	LEU	A	187	68.490	34.600	6.219	1.00	18.88

	ATOM	1239	0	LEU A	187	67.385	34.788	5.712	1.00	20.91
	ATOM	1240	N	LEU A	188	69.224	33.529	5.972	1.00	21.65
	ATOM	1241	CA	LEU A	188	68.787	32.479	5.069	1.00	24.39
	ATOM	1242	CB	LEU A	188	70.000	31.759	4.474	1.00	24.36
5	ATOM	1243	CG	LEU A	188	71.063	32.656	3.853	1.00	23.20
	ATOM	1244	CD1	LEU A	188	72.240	31.834	3.352	1.00	22.15
	ATOM	1245	CD2	LEU A	188	70.467	33.499	2.737	1.00	22.86
	ATOM	1246	С	LEU A	188	67.869	31.481	5.753	1.00	26.90
	MOTA	1247	0	LEU A	188	68.136	31.039	6.879	1.00	27.46
10	MOTA	1248	N	LEU A	189	66.786	31.135	5.058	1.00	27.05
	MOTA	1249	CA	LEU A	189	65.802	30.200	5.559	1.00	29.15
	MOTA	1250	СВ	LEU A	189	64.434	30.877	5.628	1.00	28.90
	ATOM	1251	CG	LEU A	189	64.289	32.054	6.581	1.00	26.77
	ATOM	1252	CD1	LEU A	189	62.832	32.520	6.637	1.00	28.02
15	ATOM	1253	CD2	LEU A	189	64.798	31.679	7.971	1.00	27.53
	ATOM	1254	С	LEU A	189	65.668	28.977	4.666	1.00	33.15
	ATOM	1255	0	LEU A	189	65.827	29.059	3.435	1.00	33.46
	MOTA	1256	N	ASP A	190	65.376	27.857	5.327	1.00	35.73
	ATOM	1257	CA	ASP A	190	65.108	26.609	4.632	1.00	37.59
20	MOTA	1258	CB	ASP A	190	65.798	25.424	5.338	1.00	38.82
	MOTA	1259	CG	ASP A	190	65.775	24.136	4.535	1.00	39.75
	MOTA	1260	OD1	ASP A	190	66.831	23.515	4.370	1.00	39.88
	MOTA	1261	OD2	ASP A	190	64.679	23.750	4.076	1.00	39.72
	MOTA	1262	С	ASP A	. 190	63.601	26.498	4.600	1.00	39.63
25	MOTA	1263	0	ASP A	. 190	62.945	26.557	5.634	1.00	38.67
	MOTA	1264	N	PRO A	. 191	63.054	26.347	3.345	1.00	.41.30
	ATOM	1265	CD	PRO A	. 191	63.606	26.905	2.106	1.00	43.05
	ATOM	,1266	CA	PRO A	191	61.636	26.378	3.230	1.00	42.88
	MOTA	.1267	CB	PRO P	191	61.355	25.989	1.827	1.00	43.47
30	MOTA	1268	CG	PRO A	191	62.479	26.714	1.120	1.00	44.65
	ATOM	1269	С	PRO P	191	61.091	25.558	4.271	1.00	43.67
	MOTA	1270	0	PRO A	191	60.198	25.877	5.043	1.00	45.02
	ATOM	1271	N	ASP A	192	61.712	24.392	4.198	1.00	43.63
•	ATOM	1272	CA	ASP A	A 192	61.232	23.245	4.931	1.00	43.69
35	MOTA	1273	CB	ASP A	A 192	61.357	22.022	4.086	1.00	45.58

	ATOM	1274	CG	ASP A 19	92 60.818	22.195	2.695	1.00	46.33
	ATOM	1275	OD1	ASP A 19	59.591	22.363	2.541	1.00	46.49
	ATOM	1276	OD2	ASP A 19	92 61.616	22.168	1.743	1.00	48.09
	ATOM	1277	С	ASP A 19	92 61.792	22.660	6.271	1.00	42.33
5	ATOM	1278	0	ASP A 19	92 61.192	21.674	6.684	1.00	43.45
	ATOM	1279	N	THR A 19	93 62.857	23.095	6.969	1.00	40.04
	MOTA	1280	CA	THR A 19	93 63.208	22.534	8.269	1.00	38.45
	ATOM	1281	СВ	THR A 19	93 64.684	22.092	8.356	1.00	37.80
	ATOM	1282	OG1	THR A 19	93 65.498	23.047	7.662	1.00	38.94
10	MOTA	1283	CG2	THR A 19	93 64.855	20.721	7.717	1.00	37.62
	MOTA	1284	С	THR A 19	93 62.899	23.654.	9.248	1.00	37.60
	MOTA	1285	0	THR A 19	93 62.720	23.448	10.444	1.00	37.52
	MOTA	1286	N	ALA A 19	94 62.858	24.855	8.720	1.00	35.57
	ATOM	1287	CA	ALA A 19	94 62.599	26.006	9.539	1.00	34.21
15	MOTA	1288	CB	ALA A 19	94 61.615	25.681	10.649	1.00	36.13
	ATOM	1289	С	ALA A 19	94 63.940	26.493	10.127	1.00	32.61
	ATOM	1290	0	ALA A 1	94 63.973	27.376	10.993	1.00	32.94
	ATOM	1291	N	VAL A 19	95 65.042	25.920	9.636	1.00	29.19
	MOTA	1292	CA	VAL A 1	95 66.376	26.298	10.094	1.00	25.71
20	ATOM	1293	CB	VAL A 1	95 67.415	25.237	9.725	1.00	23.91
	MOTA	1294	CG1	VAL A 1	95 68.812	25.712	10.092	1.00	24.71
	ATOM	1295	CG2	VAL A 1	95 67.104	23.922	10.420	1.00	24.73
	ATOM	1296	С	VAL A 1	95 66.791	27.640	9.486	1.00	26.18
	MOTA	1297	0	VAL A 1	95 66.454	27.934	8.332	1.00	27.87
25	MOTA	1298	N	LEU A 1	.96 67.516	28.447	10.271	1.00	21.67
	MOTA	1299	CA	LEU A 1	.96 67.980	29.752	9.838	1.00	18.05
	MOTA	1300	CB	LEU A 1	.96 67.348	30.885	10.662	1.00	17.64
	ATOM	1301	CG	LEU A 1	.96 67.930	32.299	10.469	1.00	17.61
* •	MOTA	1302	CD1	LEU A 1	196 66.867	33.352	10.714	1.00	16.49
30	ATOM	1303	CD2	LEU A 1	196 69.143	32.535	11.368	1.00	20.40
	MOTA	1304	С	LEU A 1	L96 69.484	29.830	9.893	1.00	17.95
	MOTA	1305	0	LEU A 1	196 70.118	3 29.286	10.795	1.00	16.92
	ATOM	1306	N	LYS A 1	197 70.062	30.505	8.915	1.00	17.55
	ATOM	1307	CA	LYS A 1	197 71.496	30.653	8.856	1.00	17.81
35	ATOM	1308	CB	LYS A 1	197 72.10	7 29.725	7.806	1.00	19.05

	7 TIOM	1200	CC	LYS A	107		71.753	28.267	8.014	1.00	21 12
	ATOM	1309					72.851	27.344	7.520	1.00	
	ATOM	1310		LYS A			72.434	25.880	7.619	1.00	
	MOTA	1311	CE	LYS A						1.00	•
_	ATOM	1312	NZ	LYS A			73.276	25.109	8.585		
5	ATOM	1313		LYS A			71.849	32.095	8.570	1.00	
	ATOM	1314	0	LYS A			71.160	32.778	7.795	**	20.26
	ATOM [.]	1315	N		198		72.922	32.548	9.204		18.11
	MOTA	1316	CA	LEU A			73.418	33.905	9.053		18.99
	ATOM	1317	CB	LEU A	198		74.203	34.298	10.327		19.76
10	MOTA	1318	CG	LEU A	198		73.948	35.690	10.921		19.89
•	ATOM	1319	CD1	LEU F	198		75.165	36.165	11.692	1.00	16.57
	MOTA	1320	CD2	LEU F	198		73.562	36.705	9.850	1.00	14.92
	MOTA	1321	С	LEU A	198		74.391	33.921	7.883	1.00	17.30
	MOTA	1322	0	LEU A	198		75.208	33.015	7.757	1.00	15.58
15	MOTA	1323	N	CYS A	199		74.331	34.947	7.050	1.00	15.58
	MOTA	1324	CA	CYS A	199		75.272	35.004	5.938	1.00	17.83
	MOTA	1325	CB	CYS A	A 199		74.615	34.546	4.613	1.00	14.27
	ATOM	1326	SG.	CYS A	A 199		73.261	35.610	4.074	1.00	19.47
	ATOM	1327	·C	CYS I	A 199		75.868	36.383	5.789	1.00	17.30
20	ATOM	1328	0	CYS I	A 199		75.511	37.324	6.532	1.00	19.26
	ATOM	1329	N	ASP I	A 200		76.758	36.488	4.798	i.00	15.75
	ATOM	1330	CA	ASP .	A 200	1	77.438	37.708	4.426	1.00	13.20
	ATOM	1331	CB	ASP	A 200		76.467	38.705	3.819	1.00	10.32
	ATOM	1332	CG	ASP	A 200		77.134	39.973	3.349	1.00	6.94
25	MOTA	1333	.OD1	ASP	A 200		76.421	40.968	3.160	1.00	17.09
	ATOM	1334	OD2	ASP	A 200		78.361	39.977	3.177	1.00	15.72
	ATOM	1335	С	ASP	A 200		78.272	38.329	5.543	1.00	17.58
	ATOM	1336	0	ASP	A 200		77.822	39.222	6.256	1.00	17.88
	ATOM	1337	N	PHE	A 201		79.503 ⁻	37.869	5.633	1.00	17.55
30	MOTA	1338	CA	PHE	A 201		80.459	38.349	6.598	1.00	20.60
	ATOM	1339			A 201		81.208	37.152	7.212	1.00	20.19
	ATOM	1340		PHE	A 201		80.333	36.352	8.151	1.00	20.68
	ATOM	1341			A 201		79.331		7.661	1.00	18.20
	MOTA	1342			A 201		80.497	_	9.536	1.00	20.32
35	ATOM	1343			A 201		78.501				21.23
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	ATOM	1344	CE2	PHE A	A 201	79.67 7	35.742	10.395	1.00	19.54
	ATOM	1345	CZ	PHE A	A 201	78.674	34.934	9.891	1.00	20.02
	ATOM	1346	С	PHE	A 201	81.422	39.373	5.986	1.00	20.61
	ATOM	1347	0	PHE A	A 201	82.518	39.578	6.498	1.00	21.05
5	MOTA	1348	N	GLY A	A 202	80.987	40.031	4.893	1.00	22.55
	ATOM	1349	CA	GLY A	A 202	81.808	41.041	4.226	1.00	21.39
	ATOM	1350	С	GLY A	A 202	81.992	42.289	5.059	1.00	21.03
	ATOM	1351	0	GLY A	A 202	82.936	43.038	4.873	1.00	19.70
	MOTA	1352	N	SER A	A 203	81.097	42.499	6.003	1.00	23.29
10	ATOM	1353	CA	SER A	A 203	81.179	43.643	6.897	1.00	24.09
	MOTA	1354	CB	SER A	A 203	79.785	44.251	7.056	1.00	24.42
	ATOM	1355	OG	SER A	A 203	79.469	45.139	6.002	1.00	25.73
	ATOM	1356	С	SER A	A 203	81.696	43.202	8.290	1.00	23.68
	ATOM	1357	0	SER A	A 203	81.769	44.013	9.209	1.00	26.83
15	ATOM	1358	Ν,	ALA A	A 204	81.993	41.910	8.442	1.00	23.06
	ATOM	1359	CA	ALA A	204	82.435	41.321	9.722	1.00	23.57
	MOTA	1360	CB	ALA A	A 204	82.359	39.806	9.679	1.00	21.25
	MOTA	1361	C	ALA A	A 204	83.812	41.774	10.170	1.00	23.86
	MOTA	1362	0	ALA A	A 204	84.722	41.929	9.364	1.00	25.34
20	MOTA	1363	N	LYS A	A 205	83.957	42.001	11.477	1.00	25.35
	MOTA	1364	CA	LYS A	A 205	85.227	42.468	12.029	1.00	25.22
	MOTA	1365	CB	LYS A	A 205	85.278	43.999	11.925	1.00	22.62
	ATOM	1366	CG	LYS A	A 205	86.640	44.627	12.196	1.00	23.08
	MOTA	1367	CD	LYS Z	A 205	86.596.	.46,131	11.957	1.00	24.63
25	MOTA	1368	ÇE	LYS Z	A 205	87.502	46.906	12.902	1.00	25.30
	MOTA	1369	NZ	LYS	A 205	88.938	46.568	12.721	1.00	27.91
	MOTA	1370	С	LYS I	A 205	85.413	42.062	13.488	1.00	26.41
	MOTA	1371	0	LYS	A 205	84.499	42.145	14.298	1.00	26.55
	ATOM	1372	N	GLN .	A 206	86.628	41.698	13.830	1.00	28.82
30	ATOM	1373	CA	GLN .	A 206	86.934	41.382	15.205	1.00	29.31
	MOTA	1374	CB	GLN	A 206	88.113	40.422	15.285	100	32.58
	ATOM	1375	CG	GLN	A 206	87.965	39.376	16.374	1.00	37.25
	ATOM	1376	CD	GLN	A 206	89.190	38.506	16.507	1.00	40.73
	ATOM	1377	OE1	GLN	A 206	90.207	38.912	17.088	1.00	43.91
35	MOTA	1378	NE2	GLN	A 206	89.105	37.300	15.965	1.00	43.70

	ATOM	1379	С	GLN	A	206	87.284	42.701	15.882	1.00	26.36
	ATOM	1380	0	GLN	A	206	88.311	43.291	15.588	1.00	25.43
	MOTA	1381	N	LEU	A	207	86.410	43.193	16.746	1.00	26.35
	MOTA	1382	CA	LEU	A	207	86.677	44.474	17.404	1.00	26.99
5	ATOM	1383	CB	LEU	A	207	85.415	45.060	18.048	1.00	26.08
	MOTA	1384	CG	LEU	A	207	84.203	45.273	17.119	1.00	29.98
	MOTA	1385	CD1	LEU	A	207	83.250	46.312	17.693	1.00	27.89
	ATOM	1386	CD2	LEU	A	207	84.637	45.683	15.719	1.00	28.11
	MOTA	1387	С	LEU	A	207	87.845	44.359	18.396	1.00	26.56
10	MOTA	1388	0	LEU	A	207	87.995	43.337	19.067	1.00	27.11
	ATOM	1389	N	VAL	A	208	88.684	45.399	18.448	1.00	27.33
	ATOM -	1390	CA	VAL	A	208	89.852	45.436	19.332	1.00	29.22
	MOTA	1391	CB	VÀL	A	208	91.197	45.028	18.665	1.00	30.94
	ATOM	1392	CG1	VAL	A	208	90.973	44.129	17.448	1.00	31.76
15	MOTA	1393	CG2	VAL	A	208	92.055	46.232	18.314	1.00	31.13
	MOTA	1394	C	VAL	A	208	89.948	46.776	20.063	1.00	29.36
	MOTA	1395	0	VAL	A	208	89.664	47.830	19.483	1.00	27.20
	MOTA	1396	N	ARG	A	209	90.295	46.679	21.365	1.00	30.74
	MOTA	1397	CA	ARG	A	209	90.397	47.813	22.319	1.00	30.09
20	ATOM .	1398	CB	ARG	A.	209 .	91.437	47.498	23.408	1.00	30.05
	ATOM	1399	CG	ARG	A	209	90.988	47.859	24.823	1.00	29.36
	ATOM	1400	CD	ARG	A	209	90.443	49.276	24.922	1.00	23.91
	MOTA	1401	NE	ARG	A	209	90.796	49.941	26.198	1.00	20.44
_	ATOM	1402	ĊZ	ARG	A	209	89.905	50.504	27.022	1.00-	18.05
25	ATOM	1403	NH1	ARG	A	209	88.609	50.282	26.872	1.00	11.51
	MOTA	1404	NH2	ARG	A	209	90.318	51.296	28.016	1.00	22.90
	ATOM	1405	С	ARG	A	209	90.690	49.192	21.714	1.00	30.73
	MOTA	1406	0	ARG	A	209	89.804	50.061	21.696	1.00	35.19
	MOTA	1407	N	GLY	A	210	91.928	49.435	21.303	1.00	30.36
30	MOTA	1408	CA	GLY	A	210	92.268	50.767	20.800	1.00	31.43
	ATOM	1409	С	GLY	A	210	92.263	50.913	19.282	1.00	31.78
	MOTA	1410	0	GLY	A	210	93.049	51.685	18.732	1.00	30.36
	MOTA	1411	N	GLU	A	211	91.381	50.184	18.615	1.00	30.86
	MOTA	1412	CA	GLU	A	211	91.287	50.246	17.162	1.00	29.71
35	ATOM	1413	CB	GLU	Α	211	91.453	48.851	16.576	1.00	31.43

	ATOM	1414	CG	GLU A 211	92.494	48.766	15.482	1.00	35.03
	ATOM	1415	CD	GLU A 211	92.396	47.475	14.708	1.00	36.69
	ATOM	1416	OE1	GLU A 211	93.283	46.614	14.883	1.00	39.03
	MOTA	1417	OE2	GLU A 211	91.427	47.319	13.936	1.00	37.36
5	MOTA	1418	С	GLU A 211	89.958	50.842	16.715	1.00	25.76
	ATOM	1419	0	GLU A 211	88.919	50.217	16.864	1.00	26.05
•	MOTA	1420	N.	PRO A 212	89.980	52.052	16.146	1.00	23.98
	ATOM	1421	CD	PRO A 212	91.187	52.863	15.912	1.00	25.11
	MOTA	1422	CA	PRO A 212	88.766	52.713	15.662	1.00	25.74
10	ATOM	1423	СВ	PRO A 212	89.262	54.039	15.068	1.00	25.32
	MOTA	1424	CG	PRO A 212	90.636	54.232	15.615	1.00	26.73
	ATOM	1425	С	PRO A 212	88.067	51.890	14.576	1.00	24.55
	ATOM	1426	0	PRO A 212	88.708	51.170	13.811	1.00	23.81
	MOTA	1427	N	ASN A 213	86.756	52.012	14.530	1.00	23.69
15	MOTA	1428	CA	ASN A 213	85.929	51.321	13.565	1.00	21.45
	MOTA	1429	CB	ASN A 213	85.036	50.272	14.240	1.00	21.67
	ATOM	1430	CG	ASN A 213	85.724	49.456	15.309	1.00	23.99
	MOTA	1431	OD1	ASN A 213	86.444	48.509	15.011	1.00	22.92
	ATOM	1432	ND2	ASN A 213	85.489	49.819	16.581	1.00	25.34
20	ATOM	1433	С	ASN A 213	85.045	52.347	12.887	1.00	21.95
	ATOM	1434	0	ASN A 213	84.634	53.328	13.525	1.00	18.41
	MOTA	1435	N	VAL A 214	84.737	52.133	11.593	1.00	21.29
	ATOM	1436	CA	VAL A 214	83.878	53.079	10.875	1.00	18.80
	ATOM	1437	CB	VAL A 214	83.896	52.867	9.333	1.00	20.83
25	ATOM	1438	CG1	VAL A 214	85.286	53.089	8.776		18.29
	MOTA	1439	CG2	2 VAL A 214	83.399	51.474	8.972	1.00	17.72
	ATOM	1440	С	VAL A 214	82.450	52.996	11.399	1.00	16.35
	MOTA	1441	0	VAL A 214	81.946	51.909	11.662		15.23
	MOTA	1442	N	SER A 215	81.819	54.152	11.565		17.03
30	MOTA	1443	CA	SER A 215	80.451	54.244	12.092		17.65
	ATOM	1444	CB	SER A 215	80.234	55.609	12.752		17.01
	MOTA	1445	OG	SER A 215	81.119	56.581	12.212		20.75
	MOTA	1446	С	SER A 215	79.374	54.022	11.035		18.35
	MOTA	1447	0	SER A 215	78.277	53.570			14.87
35	MOTA	1448	N	PTR A 216	79.699	54.329	9.785	1.00	19.96

	MOTA	1449	CA	PTR A 216	78.779	54.432	8.719	1.00 2	3.18
	MÖTA	1450	СВ	PTR A 216	78.923	55.195	7.630	1.00 2	24.24
	ATOM	1451	CG	PTR A 216	77.794	55.416	6.633	1.00 2	24.41
	ATOM	1452	CD1	PTR A 216	76.957	56.513	6.749	1.00 2	23.89
5	ATOM	1453	CE1	PTR A 216	75.931	56.738	5.847	1.00 2	25.55
	MOTA	1454	CD2	PTR A 216	77.573	54.531	5.571	1.00 2	24.95
	ATOM	1455	CE2	PTR A 216	76.541	54.746	4.655	1.00 2	27.09
	MOTA	1456	CZ	PTR A 216	75.718	55.852	4.802	1.00 2	26.51
	ATOM	1457	ОН	PTR A 216	74.692	56.094	3.906	1.00 2	23.68
10	ATOM	1458	С	PTR A 216	78.697	52.759	8.113	1.00 2	22.70
•	MOTA	1459	Ò	PTR A 216	79.483	52.545	7.136	1.00 2	23.40
	ATOM	1460	P	PTR A 216	73.386	55.246	3.955	1.00	25.02
	ATOM	1461	OlP	PTR A 216	72.673	55.580	2.615	1.00	26.72
	ATOM	1462	02P	PTR A 216	72.550	55.844	5.109	1.00	24.99
15	MOTA	1463	03P	PTR A 216	73.633	53.789	4.116	1.00	26.79
	MOTA	1464	N	ILE A 217	78.412	51.825	9.040	1.00	22.92
	MOTA	1465	CA	ILE A 217	78.245	50.432	8.679	1.00	22.89
	ATOM	1466	CB	ILE A 217	79.151	49.511	9.482	1.00	24.36
•	ATOM	1467	CG2	ILE A 217	80.338	49.075	8.646	1.00	24.92
20	ATOM	1468	CG1	ILE A 217	79.620	50.215	10.755	1.00	26.42
	MOTA .	1469	CD1	ILE A 217	78.508	50.527	11.726	1.00	25.66
	ATOM	1470	С	ILE A 217	76.788	50.056	8.867	1.00	22.46
	MOTA	1471	0	ILE A 217	75.904	50.924	8.917	1.00	24.48
	ATOM	1472	N	CYS A 218	76.529	48.727	8.924	1.00	23.13
25	ATOM	1473	CA	CYS A 218	75.205	48.111	9.040	1.00	24.75
	ATOM	1474	СВ	CYS A 218	74.546	48.490	10.371	1.00	24.22
	ATOM	1475	'SG	CYS A 218	75.331	47.761	11.851	1.00	27.07
	ATOM	1476	C	CYS A 218 ·	74.348	48.458	7.777	1.00	25.17
	MOTA	1477	0	CYS A 218	74.899	48.971	6.801	1.00	30.86
30	ATOM	1478	N	SER A 219	73.039	48.193	7.713	1.00	23.61
	ATOM	1479	CA	SER A 219	72.243	48.746	6.594	1.00	21.63
	MOTA	1480	СВ	SER A 219	71.262	47.789	5.922	1.00	13.51
	MOTA	1481	OG	SER A 219	70.190	.48.493	5.322	1.00	22.93
	MOTA	1482	С	SER A 219	71.469	49.806	7.342	1.00	22.86
35	MOTA	1483	8 0	SER A 219	71.084	49.549	8.473	1.00	24.73

	ATOM	1484	N	ARG A	A 220	71.224	50.983	6.779	1.00	21.86
•	ATOM	1485	CA	ARG A	A 220	70.550	52.102	7.471	1.00	22.08
	MOTA	1486	CB	ARG A	A 220	70.072	53.104	6.426	1.00	19.58
	MOTA	1487	CG	ARG A	A 220	69.553	54.403	7.038	1.00	19.73
5	ATOM	1488	CD	ARG A	A 220	68.658	55.174	6.086	1.00	21.19
	ATOM	1489	NE	ARG A	A 220	69.359	55.647	4.880	1.00	19.24
	ATOM	1490	CZ	ARG A	A 220	68.811	55.754	3.687	1.00	22.72
	ATOM	1491	NH1	ARG A	1 220	67.545	55.437	3.505	1.00	19.16
	ATOM	1492	NH2	ARG A	A 220	69.533	56.174	2.652	1.00	19.72
10.	MOTA	1493	С	ARG A	A 220	69.395	51.797	8.423	1.00	22.38
	ATOM	1494	0	ARG A	A 220	69.378	52.292	9.540	1.00	25.19
	ATOM	1495	N	TYR A	A 221	68.431	50.981	8.002	1.00	20.53
	ATOM	1496	CA	TYR A	A 221 ·	67.262	50.685	8.830	1.00	20.22
	ATOM	1497	CB	TYR A	A 221	66.239	49.867	8.042	1.00	21.19
15	ATOM	1498	CG	TYR A	A 221	65.495	50.609	6.941	1.00	24.83
	ATOM	1499	CD1	TYR A	A 221	64.514	49.960	6.207	1.00	24.53
	ATOM	1500	CE1	TYR A	A 221	63.826	50.608	5.193	1.00	27.31
	MOTA	1501	CD2	TYR'	A 221	65.773	51.938	6.629	1.00	24.67
	MOTA	1502	CE2	TYR A	A 221	65.091	52.594	5.619	1.00	27.03
20	MOTA	1503	CZ	TYR A	A 221	64.117	51.920	4.903	1.00	27.02
	ATOM	1504	ОН	TYR A	A 221	63.421	52.568	3.907	1.00	27.95
	ATOM	1505	С	TYR A	A 221 ·	67.605	49.936	10.144	1.00	19.96
	ATOM	1506	O	TYR A	A 221	66.871	50.021	11.121	1.00	17.56
	MOTA	1507	N	TYR A	A 222	68.704	49.203	10.115	1.00	16.92
25	ATOM	1508	CA	TYR A	A 222	69.162	48.374	11.222	1.00	17.59
	MOTA	1509	CB	TYR A	A 222	69.437	46.955	10.655	1.00	16.55
	MOTA	1510	CG	TYR A	A 222	68.318	46.531	9.726	1.00	17.84
	ATOM	1511	CD1	TYR A	A 222	67.135	46.032	10.241	1.00	15.19
_	MOTA	1512	CE1	TYR A	A 222	66.066	45.763	9.425	1.00	17.87
30	MOTA	1513	CD2	TYR A	A 222	68.407	46.741	8.336	1.00	17.61
	MOTA	1514	CE2	TYR A	A 222	67.340	46.451	7.499	1.00	17.42
	MOTA	1515	CZ	TYR I	A 222	66.168	45.972	8.049	1.00	20.27
	MOTA	1516	OH	TYR A	A 222	65.076	45.732	7.251	1.00	17.86
•	MOTA	1517	C.	TYR I	A 222	70.410	48.952	11.885	1.00	14.52
35	MOTA	1518	0	TYR I	A 222	71.144	48.242	12.546	1.00	18.29

	ATOM	1519	N	ARG A	A	223	70.659	50.231	11.670	1.00	13.60
	MOTA	1520	CA	ARG A	A	223	71.846	50.892	12.198	1.00	16.34
	MOTA	1521	CB	ARG A	A	223	72.176	52.051	11.286	1.00	14.55
	MOŢA	1522	CG	ARG A	A	223	73.552	52.627.	11.459	1.00	14.37
5	ATOM	1523	CD	ARG A	A	223	73.863	53.596	10.318	1.00	19.59
	MOTA	1524	NE	ARG 2	A	223	74.359	52.892	9.127	1.00	18.67
	MOTA	1525	CZ	ARG A	A	223	74.179	53.327	7.859	1.00	20.50
	ATOM	1526	NH1	ARG A	A	223	73.492	54.430	7.613	1.00	14.45
	ATOM	1527	NH2	ARG A	A	223	74.693	52.643	6.844	1.00	19.01
10	MOTA	1528	С	ARG A	A	223	71.647	51.417	13.633	1.00	16.61
	MOTA	1529	0	ARG 2	A	223	70.656	52.093	13.917 ,	1.00	17.43
	MOTA .	1530	N	ALA	A	224 .	72.609	51.109	14.506	1.00	18.18
	MOTA	1531	CA	ALA	A	224	72.582	51.543	15.927	1.00	18.38
	MOTA	1532	CB	ALA	A	224	73.711	50.884	16.686	1.00	14.89
15	ATOM	1533	С	ALA	A	224	72.704	53.055	16.042	1.00	20.36
	ATOM	1534	0	ALA	A	224	73.455	53.686	15.289	1.00	22.22
	MOTA	1535	N	PRO .	A	225	71.985	53.669	16.994	1.00	21.61
	MOTA	1536	CD	PRO .	A	225	71.087	52.998	17.959	1.00	23.19
	ATOM	1537	CA	PRO .	A	225	72.028	55.114	17.194	1.00	20.61
20	ATOM	1538	CB	PRO .	A	225	71.154	55.367	18.446	1.00	23.43
	ATOM	1539	CG	PRO .	A	225	70.894	54.023	19.050	1.00	20.97
	MOTA	1540	С	PRO .	A	225	73.437	55.664	17.383	1.00	19.98
	ATOM	1541	0	PRO	A	225	73.749.	56.744	16.870	1.00	21.76
·	ATOM	1542	N	GLU	A	226	74.297	54.942	18.109	1.00	17.57
25	ATOM	1543	CA	GLU	A	226	75.675	55.421	18.336	1.00	18.64
	ATOM	1544	CB	GLU	A	226	76.463	54.477	19.247	1.00	18.48
	ATOM	1545	CG	GLU	A	226	75.604	53.678	20.196	1.00	21.27
	ATOM	1546	CD	GLU	A	226	75.033	52.420	19.594	1.00	14.40
	ATOM	1547	OE1	GLU	A	226	73.840.	52.402	19.337	1.00	18.85
30	MOTA	1548	OE2	GLU	A	226	75,766	51.443	19.432	1.00	18.95
•	ATOM	1549	С	GLU	A	226	76.430	55.578	17.018	1.00	17.88
	ATOM	1550	0	GLU	A	226	77.238	56.487	16.856	1.00	16.85
	MOTA	1551	N	LEU	A	227	76.155	54.676	16.078	1.00	17.24
	MOTA	1552	CA	LEU	A	227	76.799	54.723	14.761	1.00	15.64
35	ATOM	1553	CB	LEU	A	227	76.282	53.558	13.910	1.00	12.39

	ATOM	1554	CG	LEU A	227	77.119	52296 ·	13 831	1.00	9.07
		1555		LEU A		78.440	52.388			10.12
	ATOM					76.339	51.080		1.00	8.78
	ATOM	1556	CD2	LEU A		76.454	56.053			10.59
5	ATOM	1557		LEU A				13.569		15.04
ے	ATOM	1558	0	LEU A		77.311		•		
	ATOM	1559	N	ire y		75.192			1.00	
	ATOM	1560	CA	ILE A		74.689	57.682	13.630		14.10
	ATOM	1561	CB	ILE A		73.152	57.723	13.726		14.29
1.0	ATOM	1562		ILE A		72.568	58.876	12.919		16.27
10	MOTA	1563		ILE A		72.572	56.384	13.248		12.90
	ATOM	1564	CD1	ILE A	228	71.062		13.299	•	10.99
	ATOM	1565	С	ILE A	228	75.347	58.910	14.301	1.00	20.58
-	MOTA	1566	0	ILE A	228	75.481	59.994	13.676	1.00	18.93
	ATOM	1567	И	PHE A	229	75.805	58.728	15.568	1.00	21.36
15	MOTA	1568	CA	PHE A	229	76.498	59.793	16.316	1.00	20.89
	ATOM	1569	CB	PHE A	229	76.331	59.595	17.837	1.00	19.68
	MOTA	1570	CG	PHE A	229	75.075	60.197	18.363	1.00	14.10
	MOTA	1571	CD1	PHE A	229	73.934	59.446	18.471	1.00	13.94
	MOTA	1572	CD2	PHE A	229	75.039	61.527	18.738	1.00	15.54
20	ATOM	1573	CE1	PHE A	229	72.763	60.003	18.949	1.00	14.85
	ATOM	1574	CE2	PHE A	229	73.881	62.093	19.219	1.00	14.22
•	ATOM	1575	CZ	PHE A	229	72.737	61.324	19.326	1.00	14.85
•	MOTA	1576	C.	PHE A	. 229	77.977	59.837	15.956	1.00	22.21
	ATOM	1577	0	PHE A	229	78.751	60.572	16.570	1.00	21.85
25	ATOM	1578	N	GLY A	230	78.369	59.050	14.937	1.00	23.72
	ATOM	1579	CA	GLY A	230	79.756	59.023	14.484	1.00	22.28
	ATOM	1580	С	GLY A	230	80.677	58.185	15.357	1.00	21.94
	ATOM	1581	0	GLY A	230	81.896	58.282	15.256	1.00	20.64
	ATOM	1582	N	ALA A	231	80.104	57.378	16.226	1.00	23.66
30	ATOM	1583	CA	ALA A	231	80.899	56.549	17.133	1.00	23.44
	ATOM	1584	CB	ALA A	A 231	79.975	55.750	18.052	1.00	24.45
	MOTA	1585	С	ALA A	A 231	81.813	55.597	16.381	1.00	22.95
	ATOM	1586	0	ALA A	A 231	81.337	54.811	15.554	1.00	23.77
	ATOM	1587	N	THR A	A 232	83.106	55.653	16.711	1.00	20.60
35	ATOM	1588	CA	THR A	A 232	84.135	54.789	16.131	1.00	22.86

	ATOM	1589	CB	THR A	232		85.356	55.607	15.681	1.00 2	24.85
	ATOM	1590		THR A			85.772	56.528	16.687	1.00	
	ATOM	1591		THR A			85.123	56.392	14.396	1.00 2	
	ATOM	1592	C	THR A			84.555	53.706 .		1.00 2	
5	ATOM	1593		THR A			85.235	52.744	16.777	1.00	
J	ATOM	1594	N	ASP A		•	84.110	53.873	18.376	1.00	22.55
	ATOM	1595	CA	ASP A			84.381	52.930	19.470	1.00	19.98
	ATOM	1596	СВ	ASP A			85.078	53.649	20.640	1.00	
	ATOM	1597	CG	ASP A			85.181	52.837	21.952	1.00	26.33
10	ATOM	1598		ASP A			85.760	53.378.	22.917	1.00	26.39
,	ATOM	1599		ASP A		-	84.685	51.687	22.016	1.00	22.93
	ATOM	1600	С	ASP A			83.059	52.339	19.886	1.00	17.40
	ATOM	1601	0	ASP A	233		82.259	52.976	20.577	1.00	19.65
	ATOM	1602	N	TYR A	234		82.803	51.144	19.399	1.00	15.12
15	ATOM	1603	CA	TYR F	A 234		81.563	50.485	19.662	1.00	11.50
	ATOM	1604	СВ	TYR A	A 234		80.512	50.868	18.619	1.00	19.52
	ATOM	1605	CG	TYR A	A 234		80.930	50.570	17.186	.1.00	20.59
	MOTA	1606	CD1	TYR A	A 234		80.771	49.299	16.656	1.00	22.28
	ATOM	1607	CE1	TYR A	A 234		81.122	49.021	15.339	1.00	26.03
20	MOTA	1608	CD2	TYR A	A 234		81.458	51.566	16.374	1.00	20.66
	ATOM	1609	CE2	TYR A	A 234		81.818	51.301	15.053	1.00	24.62
	ATOM	1610	CZ	TYR I	A 234		81.642	50.028	14.543	1.00	24.61
	MOTA	1611	ОН	TYR	A 234		81.992	49.752	13.244	1.00	26.95
	MOTA	1612	С	TYR .	A 234		81.754	48.998	19.778	1.00	7.69
25	MOTA	1613	0	TYR	A 234		82.839	48.483	19.622	1.00	11.49
•	ATOM	1614	N	THR	A 235		80.724	48.307	20.128	1.00	8.06
	MOTA	1615	CA	THR	A 235	•	80.872	46.896	20.355	1.00	9.69
	MOTA	1616	CB	THR	A 235		,80.733	46.652	21.885	1.00	11.03
	MOTA	1617	OG	1 THR	A 235		79.364	46.654	22.225	1.00	8.81
30	ATOM	1618	CG	2 THR	A 235		81.403	47.714	22.735		
	MOTA	1619	C	THR	A 235)	79,809	46.101	19.661		11.93
	MOTA	1620	0	THR	A 235	5	78.992	46.638	18.932		15.94
	MOTA	1621	. N	SER	A 236	5	79.846	44.807			16.37
	MOTA	1622	CP	SER	A 236	5	78.943	43.800	19.422		16.47
35	ATOM	1623	3 CE	SER	A 236	5	79.388	42.436	19.914	1.00	17.79

	ATOM	1624	OG	SER A 236	80.708	42.187	19.457	1.00 23.99
	ATOM	1625	С	SER A 236	77.485	44.056	19.732	1.00 16.40
	MOTA	1626	0	SER A 236	76.613	43.391	19.145	1.00 15.77
	ATOM	1,627	N	SER A 237	77.203	.45.033	20.625	1.00 16.08
5	ATOM	1628	CA	SER A 237	75.805	45.386	20.967	1.00 11.57
	ATOM	1629	CB	SER A 237	75.718	46.324	22.176	1.00 8.80
	ATOM	1630	OG	SER A 237	76.688	47.342	22.069	1.00 9.16
	ATOM	1631	C	SER A 237	75.123	46.065	19.768	1.00 10.30
	ATOM	1632	0	SER A 237	73.898	46.129	19.703	1.00 7.31
10	ATOM	1633	N	ILE A 238	75.914	46.546	18.803	1.00 11.34
	ATOM	1634	CA	ILE A 238	75.259	47.142	17.602	1.00 14.03
	ATOM	1635	ĊB	ILE A 238	76.223	47.862	16.625	1.00 14.92
	MOTA	1636	CG2	ILE A 238	76.952	49.028	17.293	1.00 14.36
	MOTA	1637	.CG1	ILE A 238	77.197	46.891	15.967	1.00 13.71
15	ATOM	1638	CD1	ILE A 238	77.847	47.457	14.706	1.00 15.09
	ATOM	1639	С	ILE A 238	74.478	46.039	16.869	1.00 10.92
	ATOM	1640	0	ILE A 238	73.360	46.251	16.437	1.00 14.44
	ATOM	1641	N	ASP A 239	75.053	44.828	16.796	1.00 11.90
	ATOM	1642	CA	ASP A 239	74.359	43.686	16.165	1.00 12.25
20	ATOM	1643	CB	ASP A 239	75.237	42.412	16.174	1.00 10.53
	ATOM	1644	CG	ASP A 239	76.350	42.470	15.144	1.00 12.86
	ATOM	1645	OD1	ASP A 239	76.333	43.412	14.319	1.00 13.57
	ATOM	1646	OD2	ASP A 239	77.244	41.584	15.165	1.00 13.48
	ATOM ·	1647	C	ASP A 239	73.047	43.422	16.859	1.00 14.25
25	ATOM	1648	0	ASP A 239	72.034	43.071	16.204	1.00 14.57
•	ATOM	1649	N	VAL A 240	73.045	43.626	18.220	1.00 13.55
	ATOM	1650	CA.	VAL A 240	71.833	43.435	19.024	1.00 7.80
	ATOM	1651	СВ	VAL A 240	72.101	43.523	20.575	1.00 9.66
	ATOM	1652	CG1	VAL A 240	70.786	43.446	21.328	1.00 5.00
30	ATOM	1653	CG2	VAL A 240	73.036	42.420	21.023	1.00 9.17
	MOTA	1654	С	VAL A 240	70.749	44.429	18.640	1.00 5.00
	ATOM	1655	0	VAL A 240	69.593	44.071	18.522	1.00 9.41
	ATOM	1656	N	TRP A 241 ·	71.114	45.677	18.441	1.00 8.68
	ATOM	1657	CA	TRP A 241	70.115	46.682	18.039	1.00 8.70
35	MOTA	1658	CB	TRP A 241	70.785	48.063	17.942	1.00 12.59

	ATOM	1659	CG	TRP A 241	69.907	49.159	17.376	1.00 1	.3.08
	MOTA	1660	CD2	TRP A 241	69.086	50.093	18.105	1.00 1	7.91
	MOTA	1661	CE2	TRP A 241	68.435	50.922	17.145	1.00 1	L6.74
•	ATOM	1662	CE3	TRP A 241	68.824	50.309 .	19.466	1.00	L5.70
5	ATOM [.]	1663	CD1	TRP A 241	69.738	49.474	16.053	1.00	16.26
	ATOM	1664	NE1	TRP A 241	68.841	50.515	15.916	1.00	15.52
	ATOM	1665	CZ2	TRP A 241	67.552	51.940	17.507	1.00	19.78
	ATOM	1666	CZ3	TRP A 241	67.952	51.317	19.820	1.00	17.55
	MOTA	1667	CH2	TRP A 241	67.323	52.123	18.847	1.00	19.91
10	ATOM	1668	С	TRP A 241	69.501	46.257	16.672	1.00	9.05
	MOTA	1,669	0	TRP A 241	68.294	46.321	16.466	1.00	8.77
	MOTA	1670	N	SER A 242	70.357	45.787	15.756	1.00	9.89
	ATOM	1671	CA	SER A 242	69.900	45.326	14.419	1.00	11.70
	ATOM	1672	CB	SER A 242	71.097	44.938	13.521	1.00	5.00
15	ATOM	1673	OG	SER A 242	71.927	46.063	13.328	1.00	7.55
	MOTA	1674	С	SER A 242	68.926	44.177	14.578	-1.00	11.06
	ATOM	1675	0	SER A 242	67.824	44.224	14.029	1.00	13.94
	ATOM	1676	N	ALA A 243	69.305	43.169	15.398	1.00	13.36
	MOTA	1677	CA	ALA A 243	68.402	42.036	15.672	1.00	14.87
20	MOTA	1678	CB	ALA A 243	69.036	41.047	16.635	1.00	16.56
	ATOM	1679	С	ALA A 243	67.075	42.532	16.211	1.00	15.72
	ATOM	1680	0	ALA A 243	66.005	42.050	15.816	1.00	17.54
	MOTA	1681	N	GLY A 244	. 67.130	43.540	17.093	1.00	17.52
	ATOM	1682	CA	GLY A 244 .	65.897	44.097	17.620	1.00	16.24
25	MOTA	1683	C	GLY A 244	65.090	44.768	16.518	1.00	16.45
	MOTA	1684	0	GLY A 244 ·	63.877	44.692	16.493	1.00	14.27
	ATOM	1685	N	CYS A 245	65.786	45.411	15.585	1.00	18.79
	ATOM	1686	CA	CYS A 245	65.118	46.062	14.447	1.00	19.45
	MOTA	1687	СВ	CYS A 245	66.139	46.841	13.614	1.00	16.90
30	MOTA	1688	SG	CYS A 245	66.564	48.451	14.319	1.00	17.99
	MOTA	1689	С	CYS A 245	64.407	44.993	13.608	1.00	17.15
٠	ATOM	1690	0	CYS A 245	63.258	45.147	13.238	1.00	18.70
	MOTA	1691	N	VAL A 246	65.078	43.872	13.389	1.00	17.86
	MOTA	1692	CA	VAL A 246	64,478	42.754	12.668	1.00	19.17
35	ATOM	1693	CB	VAL A 246	65.465.	41.586	12.519	1.00	16.94

•	ATOM	1694	CG1	VAL A	246	64.803	40.416	11.810	1.00 16.17
	ATOM	1695	CG2	VAL A	246	66.713	42.023	11.797	1.00 20.27
	ATOM	1696	С	VAL A	246	63.232	42.244	13.386	1.00 21.86
	ATOM	1697 '	0	VAL A	246	62.177	42.028	12.758	1.00 22.61
5 .	ATOM	1698	N	LEU A	247	63.336	42.044	14.726	1.00 22.24
	ATOM	1699	CA	LEU A	247 ·	62.189	41.556	15.520	1.00 17.75
	ATOM	1700	СВ	LEU A	247	62.556	41.563	17.018	1.00 21.43
	ATOM	1701	CG	LEU A	247	61.857	40.556	17.931	1.00 21.52
	MOTA	1702	CD1	LEUA	247	61.533	41.174	19.293	1.00 21.62
10	ATOM	1703	CD2	LEU A	247	60.624	39.960	17.283	1.00 19.10
	ATOM	1704	С	LEU A	247	60.984	42.438	15.331	1.00 16.58
	ATOM ·	1705	Ο.	LEU A	247	59.882	41.963	15.074	1.00 17.00
	ATOM	1706	N	ALA A	248	61.190	43.732	15.508	1.00 17.51
-	ATOM	1707	CA	ALA A	248	60.117	44.718	15.399	1.00 17.76
15	ATOM	1708	CB	ALA A	248	60.675	46.096	15.718	1.00 13.92
	ATOM	1709	С	ALA A	248	59.479	44.694	14.001	1.00 19.04
	ATOM	1710	0	ALA A	248	58.248	44.674	13.868	1.00 19.92
	MOTA	1711	N	GLU A	249	60.326	44.675	12.956	1.00 19.92
	ATOM	1712	CÄ	GLU A	249	59.836	44.623	11.570	1.00 18.88
20	MOTA	1713	CB	GLU A	249	61.017	44.571	10.588	1.00 22.05
	MOTA	1714	CG	GLU A	249	60.629	44.870	9.143	1.00 24.95
	ATOM	1715	CD	GLU A	249	61.815	44.888	8.200	1.00 26.40
•	ATOM	1716	OE1	GLU A	249	62.860	45.461	8.573	1.00 27.15
•	MOTA	1717	OE2	GLU A	249 .	61:699	44.330	7.086	1.00 26.13
25	ATOM	1718	C	GLU A	249	58.942	43.404	11.383	1.00 16.29
	ATOM	1719	0	GLU A	249	57.857	43,488	10.842	1.00 16.64
	ATOM	1720	N	LEU A	250	59.391	42.265	11.872	1.00 18.94
	ATOM	1721	CA	LEU A	250	58.611	41.041	11.765	1.00 19.63
	ATOM	1722	CB	LEU A	250	59.421	39.855	12.227	1.00 21.77
30	ATOM	1723	CG	LEU A	250	60.508	39.410	11.255	1.00 21.90
	ATOM	1724	CD1	LEU A	250	61.205	38.171	11.789	1.00 22.15
	ATOM	1725	CD2	LEU A	250	59.894	39.138	9.882	1.00 20.69
	MOTA	1726	С	LEU A	250	57.257	41.102	12.453	1.00 21.42
_	ATOM	1727	0	LEU A	. 250	56.302	40.428	12.029	1.00 19.97
35	ATOM	1728	N	LEU A	251	57.153	41.914	13.513	1.00 22.22

	ATOM ATOM	1729	CA	LEU A 251	55.886	42.050	14.226	1.00 22.60
	MOTA	1770						
		1730	CB	LEU A 251	56.111	42.386	15.712	1.00 21.94
	ATOM	1731	CG	LEU A 251	57.047	41.470	16.505	1.00 23.22
	ATOM	1732	CD1	LEU A 251	57.607	42.223 .	17.699	1.00 22.21
5	ATOM	1733	CD2	LEU A 251	56.323	40.209	16.955	1.00 20.09
	MOTA	1734	С	LEU A 251	55.039	43.150	13.598	1.00 22.16
	ATOM	1735	0	LEU A 251	53.833	43.063	13.578	1.00 21.07
	MOTA	1736	N	LEU A 252	55.699	44.193	13.109	1.00 24.69
	ATOM	1737	CA	LEU A 252	55.026	45.333	12.497	1.00 27.50
10	ATOM	1738	CB	LEU A 252	55.990	46.519	12.422	1.00 28.83
	ATOM	1739	CG	LEU A 252	55.884	47.597	13.506	1.00 31.65
	ATOM	1740	CD1	LEU A 252	54.636	47.423	14.368	1.00 29.59
	MOTA	1741	CD2	LEU A 252	57.143	47.620	14.358	1.00 30.57
	ATOM	1742	C	LEU A 252	54.532	45.033	11.082	1.00 28.49
15	ATOM	1743	0	LEU A 252	53.475	45.518	10.676	1.00 29.11
	MOTA	1744	N	GLY A 253	55.328	44.283	10.320	1.00 29.33
	MOTA	1745	CA	GLY A 253	54.978	43.997	8.933	1.00 29.31
	ATOM	1746	С	GLY A 253 ·	55.609	45.024	8.000	1.00 30.52
	ATOM	1747	0	GLY A 253	55.243	45.121	6.829	1.00 31.13
20	MOTA	1748	N	GLN A 254	56.567	45.795	8.548	1.00 31.15
	ATOM	1749	CA	GLN A 254	57.308	46.846	7.841	1.00 30.85
	ATOM	1750	CB	GLN A 254	56.375	47.991	7.462	1.00 31.46
	MOTA	1751	CG	GLN A 254	55.850	48.778	8.651	1.00 30.44
	MOTA	1752	CD	GLN A 254	54.831	49.815	8.251	1.00 29.54
25	ATOM	1753	OE1	GLN A 254	55.153	50.984	8.096	1.00 30.99
	MOTA.	1754	NE	2 GLN A 254	53.591	49.391	8.089	1.00 32.26
	MOTA	1755	С	GLN A 254	58.416	47.378	8.747	1.00 30.06
	ATOM	1756	0	GLN A 254	58.281	47.323	9,967	1.00 31.81
	MOTA	1757	N	PRO A 255	59.525	47.896	8.182	1.00 28.75
30	MOTA	1758	CD	PRO A 255	59.786	48.003	6.736	1.00 29.77
	MOTA	1759	CA	PRO A 255	60.639	48.422	8.978	1.00 27.17
	MOTA	1760	СВ	PRO A 255	61.503	49.146	7.955	1.00 28.27
	ATOM	1761	CG	PRO A 255	61.229	48.421	6.674	1.00 30.04
	MOTA	1762	С	PRO A 255	60.166	49.386	10.059	1.00 25.98
35	ATOM	1763	0	PRO A 255	59.328	50.262	9.814	1.00 24.39

	MOTA	1764	N	ILE A	256	60.699	49.214	11.265	1.00 23.84
	MOTA	1765	CA	ILE A	256	60.301	50.071	12.381	1.00 20.82
	MOTA	1766	CB	ILE A	256	60.640	49.441	13.753	1.00 18.45
	MOTA	1767	CG2	ILE A	256	62.134	49.177 .	13.867	1.00 14.74
5 .	MOTA	1768	CG1	ILE A	256	60.145	50.352	14.887	1.00 20.07
	MOTA	1769	CD1	ILE A	256	59.894	49.626	16.196	1.00 22.63
	ATOM	1770	C	ILE A	256	60.849	51.496	12.267	1.00 18.31
	MOTA	1771	0	ILE A	256	60.143	52.459	12.578	1.00 19.96
	ATOM	1772	N	PHE A	257	62.092	51.623	11.832	1.00 .17.97
10	MOTA	1773	CA	PHE A	257	62.735	52.925	11.683	1.00 19.27
	MOTA	1774	CB	PHE A	257	63.953	53.041.	12.641	1.00 20.54
	MOTA	1775	CG	PHE A	257	63.683	52.674	14.091	1.00 18.05
	ATOM	1776	CD1	PHE A	257	62.675	53.297	14.806	1.00 18.44
	ATOM	1777	CD2	PHE A	257	64.462	51.729	14.740	1.00 19.25
15	ATOM	1778	CE1	PHE A	257	62.449	52.982	16.145	1.00 19.85
	ATOM	1779	CE2	PHE A	257	64.235	51.405	16.083	1.00 19.59
	ATOM	1780	CZ	PHE A	257	63.229	52.038	16.779	1.00 14.97
	ATOM	1781	C	PHE A	257	63.194	53.151	10.217	1.00 19.61
	MOTA	1782	0	PHE A	257	64.343	52.926	9.880	1.00 19.87
20	MOTA	1783	N	PRO A	258	62.297	53.588	9.329	1.00 21.18
	ATOM	1784	CD	PRO A	258	60.880	53.883	9.604	1.00 22.67
	ATOM	1785	CA	PRO A	258	62.632	53.821	7.908	1.00 24.51
	ATOM	1786	CB	PRO A	258	61.266	53.704	7.242	1.00 22.28
	MOTA	1787	CG	PRO A	258	60.350	54.313	8.249	1.00.25.70
25	MOTA	1788	С	PRO A	258	63.204	55.207	7.656	1.00 23.60
•	MOTA	1789	0	PRO A	258	62.481	56.116	7.287	1.00 25.61
	MOTA	1790	N	GLY A	259	64.496	55.361	7.842	1.00 26.01
	MOTA	1791	CA	GLY A	259	65.120	56.657	7.608	1.00 29.65
	MOTA	1792	С	GLY A	259	65.385	56.916	6.121	1.00 31.04
30	MOTA	1793	0	GLY A	259	65.717	55.985	5.389	1.00 30.01
	MOTA	1794	N	ASP A	260	65.232	58.181	5.684	1.00 31.88
	ATOM	1795	CA	ASP A	260	65.450	58.560	4.282	1.00 33.04
	ATOM	1796	CB	ASP A	260	64.452	59.635	3.814	1.00 33.94
	MOTA	1797	CG	ASP A	. 260	64.645	60.997	4.466	1.00 35.58
35	MOTA	1798	OD1	ASP A	260	65.719	61.250	5.023	1.00 35.78

	MOTA	1799	OD2	ASP A	Ą	260	(63.713	61.819	4.407	1.00	38.52
	MOTA	1800	С	ASP A	A	260	(66.897	58.962	4.008	1.00	32.63
	MOTA	1801	0	ASP A	A	260	1	67.258	59.313	2.875	1.00	33.30
•	MOTA	1802	N	SER A	A	261	•	67.709	58.884	5.056	1.00	31.36
5	MOTA	1803	CA	SER A	A °	261	+	69.145	59.189	5.043	1.00	30.25
	ATOM	1804	CB	SER A	A	261		69.435	60.692	4.935	1.00	32.71
	MOTA	1805	OG	SER A	A	261		69.062	61.392	6.117	1.00	33.13
	ATOM	1806	С	SER A	A	261	+	69.769	58.623	6.308	1.00	28.76
	MOTA	1807	0	SER A	A	261		69.058	58.090	7.146	1.00	28.26
10	ATOM	1808	N	GLY A	A	262	•	71.092	58.725	6.423	1.00	28.70
	ATOM	1809	CA	GLY A	A	262		71.808	58.208	7.576	1.00	25.78
	ATOM	1810	С	GLY 2	A	262		71.576	59.021	8.851	1.00	26.60
	ATOM	1811	0	GLY Z	A	262		71.723	58.491	9.959	1.00	23.39
	ATOM	1812	N	VAL 2	A	263		71.209	60.304	8.681	1.00	25.15
15	ATOM	1813	CA	VAL .	A	263		70.944	61.211	9.799	1.00	23.70
	ATOM	1814	CB	VAL .	A	263		71.429	62.643	9.489	1.00	24.57
	MOTA	1815	CG1	VAL .	A	263	-	70.777	63.679	10.400	1.00	26.49
	MOTA	1816	CG2	VAL .	A	263		72.940	62.719	9.585	1.00	24.46
	MOTA	1817	С	VAL .	A	263		69.463	61.213	10.126	1.00	23.60
20	ATOM	1818	0	VAL	A	263		69.074	61.339	11.298	1.00	23.21
	ATOM	1819	N '	ASP	A	.264		68.635	61.037 .	9.086	1.00	18.63
	MOTA	1820	CA	ASP	A	264		67.189	60.977	9.243	1.00	16.12
	ATOM	1821	CB	ASP	A	264		66.516	61.007	7.873	1.00	16.93
	MOTA	1822	CG	ASP	A	264		65.023	61.085	7.967	1.00	15.99
25	ATOM	1823	OD1	ASP	A	264		64.518	62.131	8.361	1.00	23.33
	MOTA	1824	OD2	ASP	A	264		64.353	60.101	7.645	1.00	21.38
	MOTA	1825	С	ASP	A	264		66.799	59.688	9.956	1.00	14.34
	ATOM	1826	0	ASP	A	264		65.708	59.566	10.512	1.00	11.71
	ATOM	1827	N	GLN	A	265 ,		67.712	58.739	9.919	1.00	13.50
30	ATOM	1828	CA	GLN	A	265		67.543	57.453	10.551	1.00	16.78
	ATOM	1829	CB	GLN	A	265		68.761	56.593	10.222	1.00	15.08
	ATOM	1830	CG	GLN	A	265		68.718	55.172	10.751	1.00	22.06
•	ATOM	1831	CD	GLN	A	265		67.534	54.379	10.241	1.00	24.38
	MOTA	1832	OE1	GLN	A	265		66.925	54.718	9.216	1.00	26.93
35	MOTA	1833	NE2	GLN	A	265		67.195	53.317	10.957	1.00	25.58

		ATOM	1834	С	GLN	A	265	67.420	57.667	12.082	1.00	18.49
		ATOM	1835	0	GLN	A	265	66.649	56.981	12.750	1.00	17.65
		ATOM	1836	N	LEU	A	266	68.158	58.660	12.595	1.00	20.41
		MOTA	1837	CA	LEU	A	266	68.120	59.024	14.015	1.00	23.21
	5	ATOM	1838	CB	LEU	A	266	69.293	59.962	14.385	1.00	19.14
		MOTA	1839	CG	LEU	A	266	69.499	60.258	15.898	1.00	22.99
		ATOM	1840	CD1	LEU	A	266	69.548	58.966	16.726	1.00	13.89
		ATOM	1841	CD2	LEU	A	266	70.754	61.085	16.119	1.00	19.84
		ATOM	1842	C	LEU	A	266	66.774	59.677	14.342	1.00	24.24
	10	MOTA	1843	0	LEU	A	266	66.171	59.387	15.394	1.00	25.95
		ATOM	1844	N	VAL	A	267	66.284	60.541	13.428	1.00	20.54
		MOTA	1845	CA	VAL	A	267	64.997	61.209	13.623	1.00	21.02
		MOTA	1846	CB	VAL	A	267	64.661	62.250	12.512	1.00	22.65
		ATOM	1847	CG1	VAL	A	267	63.242	62.786	12.679	1.00	20.94
	15	MOTA	1848	CG2	. VAL	A	267	65.659	63.397	12.492	1.00	23.85
		MOTA	1849	С	VAL	A	267	63.867	60.202	13.712	1.00	21.30
		ATOM	1850	0	VAL	A	267	62.916	60.389	14.487	1.00	21.41
		ATOM	1851	N	GLU	A	268	63.961	59.136	12.904	1.00	21.14
	-	ATOM	1852	CA	GLU	A	268	62.940	58.087	12.880	1.00	21.32
	20	ATOM	1853	CB	GLU	A	268	63.188	57.109	11.714	1.00	20.56
		ATOM	1854	CG	GLU	A	268	62.780	57.634	10.337	1.00	19.52
		ATOM	1855	CD	GLU	Α	268	61.323	58.007	10.270	1.00	15.74
	•	АТОЙ	1856	OE1	GLU	A	268	61.022	59.170	9.958	1.00	19.10
		MOTA	1857	OE2	ĞLU	A	268	60.483	57.137	10.542	1.00	21.33
	25	ATOM .	1858	С	GLU	A	268	62.947	57.315	14.203	1.00	20.77
		MOTA	1859	0	GLU	A	. 268	61.900	56.973	14.744	1.00	21.32
		MOTA	1860	N	ILE	A	. 269	64.133	57.042	14.704	1.00	20.21
		MOTA	1861	CA	ILE	P	269	64.272	56.315	15.965	1.00	22.93
		MOTA	1862	CB	ILE	<u> </u>	269	65.753	56.013	16.272	1.00	21.57
	30	MOTA	1863	CG2	2 ILE	E P	269	65.916	55.490	17.704	1.00	21.70
		MOTA	1864	CG1	LILE	E P	269	66.320	55.012	15.261	1.00	16.65
•		ATOM	1865	CD	LIL	E P	A 269	67.827	54.977	15.231	1.00	12.77
		ATOM	1866	С	ILI	E P	A 269	63.680	57.149	17.106	1.00	22.44
•		ATOM	1867	0	IL	E A	A 269	62.822	56.684	17.835	1.00	22.07
	35	ATOM	1868	N	IL	E <i>1</i>	A 270	64.150	58.393	17.208	1.00	24.28

	MOTA	1869	CA	ILE .	A 2	70	63.711	59.347	18.209	1.00	26.56
	MOTA	1870	СВ	ILE .	A 2	70	64.358	60.727	17.967	1.00	24.36
	ATOM	1871	CG2	ILE .	A 2	70	63.698	61.791	18.831	1.00	27.65
	ATOM	1872	CG1	ILE	A 2	70	65.853	60.652 .	18.264	1.00	20.73
5	ATOM	1873	CD1	ILE	A 2	70	66.567	61.983	18.215	1.00	18.62
	MOTA	1874	С	ILE	A 2	70	62.195	59.480	18.234	1.00	29.28
	MOTA	1875	0	ILE	A 2	70	61.588	59.653	19.301	1.00	28.79
	MOTA	1876	N	LYS	A 2	71	61.591	59.401	17.054	1.00	29.05
	ATOM	1877	CA	LYS	A 2	71	60.144	59.519	16.903	1.00	28.68
10	ATOM	1878	СВ	LYS	A 2	71	59.815	59.543	15.402	1.00	32.12
	ATOM	1879	CG	LYS	A 2	71	58.345	59.527	15.052	1.00	35.46
	ATOM	1880	CD	LYS	A 2	71	58.159	59.612	13.536	1.00	39.81
	ATOM	1881	CE	LYS	A 2	71	58.964	60.767	12.942	1.00	39.81
	ATOM	1882	NZ	LYS	A 2	71	58.903	60.792	11.455	1.00	42.86
15	MOTA	1883	С	LYS	A 2	71	59.414	58.393	17.625	1.00	28.22
	MOTA	1884	0	LYS	A 2	71	58.219	58.488	17.897	1.00	26.93
	MOTA	1885	N	VAL	A 2	72	60.144	57.334	17.950	1.00	28.27
	ATOM	1886	CA	VAL	A 2	72	59.578	56.195	18.655	1.00	27.38
	ATOM	1887	CB	VAL	A 2	72	59.837	54.878	17.904	1.00	27.95 .
20	MOTA	1888	CG1	VAL	A 2	72	59.334	53.688	18.710	1.00	27.27
	MOTA	1889	CG2	VAL	A 2	:72	59.184	54.908	16.531	1.00	26.96
	ATOM	1890	С	VAL	A 2	272	60.123	56.080	20.091	1.00	27.25
	ATOM	1891	0	JAV	A 2	272	59.361	55.807	21.012	1.00	28.50
	ATOM	1892	N	LEU	A 2	?73·	61:439	56.266	20.263	1.00	25.88
25 ·	MOTA	1893	CA	LEU	A. 2	273	62.096	56.160	21.573	1.00	25.89
	MOTA	1894	CB	LEU	A 2	273 .	63.515	55.612	21.394	1.00	22.17
	MOTA	1895	CG	LEU	A 2	273	63.671	54.117	21.116	1.00	21.67
	ATOM	1896	CD1	LEU	A 2	273.	65.066	53.656	21.519	1.00	23.34
	ATOM	1897	CD2	LEU	A 2	273	62.614	53,308	21.842	1.00	22.69
30	ATOM	1898	С	LEU	A 2	273	62.198	57.510	22.304	1.00	27.83
	ATOM	1899	0 .	LEU	A 2	273	62.869	57.608	23.342	1.00	30.31
	MOTA	1900	N	GLY	A	274	61.577	58.545.	21.746		26.13
	MOTA	1901	CA	GLY	A	274	61.641	59.866	22.327	1.00	23.58
	MOTA	1902	С	GLY	A	274	63.038	60.415	22.272	1.00	23.20
35	ATOM	1903	0	GLY	A	274	63.972	59.679	22.001	1.00	24.94

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	ATOM	1904	N	THR A	A 275	63.194	61.706	22.523	1.00	23.62	
	ATOM	1905	CA	THR P	A 275	64.515	62.318	22.484	1.00	25.71	
•	ATOM	1906	CB	THR A	A 275	64.440	63.805	22.849	1.00	24.96	
	ATOM	1907	OG1	THR A	A 275	63.379	64.466 .	22.191	1.00	27.34	
5 .	ATOM	1908	CG2	THR A	A 275	65.714	64.569	22.589	1.00	24.20	
	ATOM .	1909	C	THR A	A 275	65.469	61.619	23.445	1.00	27.31	
	ATOM	1910	0	THR A	A 275	65.094	61.315	24.574	1.00	30.40	
	ATOM	1911	N	PRO A	A 276	66.723	61.365	23.019	1.00	27.93	
	ATOM	1912	CD	PRO A	A 276	67.267	61.693	21.677	1.00	26.71	
10	ATOM	1913	CA	PRO A	A 276	67.717	60.727	23.868	1.00	27.45	
	ATOM	1914	СВ	PRO A	A 276	68.783	60.280	22.871	1.00	27.30	
	ATOM	1915	CG	PRO A	A 276	68.711	61.288	21.774	1.00	25.15	
	ATOM	1916	С	PRO A	A 276	68.307	61.745	24.845	1.00	29.86	
	ATOM	1917	0	PRO I	A 276	68.482	62.925	24.497	1.00	28.23	
15	ATOM	1918	N	THR A	A 277	68.617	61.296	26.068	1.00	28.52	
	ATOM	1919	CÀ	THR A	A 277	69.191	62.194	27.067	1.00	28.53	
	ATOM	1920	CB	THR A	A 277	68.948	61.688	28.498	1.00	27.08	•
	ATOM	1921	OG1	THR .	A 277	69.701	60.528	28.751	1.00	26.20	
	MOTA	1922	CG2	THR A	A 277	67.504	61.380	28.816	1.00	26.96	
20	MOTA	1923	C	THR I	A 277	70.675	62.348	26.833	1.00	29.01	
	MOTA	1924	0	THR 2	A 277	71.296	61.502	26.175	1.00	29.53	
	ATOM	1925	N	ARĠ	A 278	71.246	63.415	27.386	1.00	29.35	
•	ATOM	1926	CA	ARG :	A 278	72.676	63.671	27.257	.1.00	31.97	
	ATOM	1927	CB	·ARG	A 278	73.041	64.986	27.950	1.00	35.10	
25	ATOM	1928	CG	ARG .	A 278	74.393	65.536	27.537	1.00	39.53	
	ATOM	1929	CĐ	ARG	A 278	75.396	65.452	28.681	1.00	44.28	
	ATOM	1930	NE	ARG	A 278	75.067	66.386	29.763	1.00	45.67	
	ATOM	1931	CZ	ARG.	A 278	75.973	67.048	30.493	1.00	47.63	
	MOTA	1932	NHI	ARG	A 278	77.280	66.820	30.338	1.00	48.34	
30	ATOM	1933	NH2	ARG	A 278	75.566	67.937	31.396	1.00	48.46	
	ATOM	1934	С	ARG	A 278	73.490	62.515	27.850	1.00	31.24	
	ATOM	1935	0	ARG	A 278	74.581	62.190	27.359	1.00	32.03	
	ATOM	1936	N	GLU	A 279	72.937	61.888	28.895	1.00	29.06	
	ATOM	1937	CA	GLU	A 279	73.574	60.749	29.555	1.00	28.36	
35	ATOM	1938	CB	GLU	A 279	72.823	60.403	30.847	.1.00	29.62	

		MOTA	1939	CG	GLU A	A 279	73.360	59.189	31.601	1.00	33.37
		MOTA	1940	CD	GLU A	A 279	72.382	58.696	32.669	1.00	37.46
		ATOM	1941	OE1	GLU Z	A 279	72.139	57.462	32.746	1.00	38.36
		MOTA	1942	OE2	GLU Z	A 279	71.849	59.544	33.423	1.00	37.26
	5	MOTA	1943	С	GLU A	A 279	73.581	59.537	28.620	1.00	24.06
	٠	ATOM	1944	0	GLU Z	A · 279	74.582	58.865	28.468	1.00	23.16
		ATOM	1945	N	GLN I	A 280	. 72.457	59.281	27.984	1.00	23.18
		MOTA	1946	CA	GLN A	A 280	72.367	58.170	27.045	1.00	23.13
		MOTA	1947	CB	GLN Z	A 280	70.948	58.033	26.532	1.00	21.72
	10	ATOM	1948	CĠ	GLN A	A 280	69.976	57.424	27.513	1.00	19.01
		MOTA	1949	CD	GLN 3	A 280	68.561	57.553	27.033	1.00	16.19
		MOTA	1950	OE1	GLN 3	A 280	68.175	58.582	26.491	1.00	20.58
		ATOM	1951	NE2	GLN .	A 280	67.772	56.513	27.225	1.00	19.66
		ATOM	1952	С	GLN .	A 280	73.322	58.407	25.869	1.00	22.75
	15	ATOM	1953.	0	GLN .	A 280	73.922	57.476	25.365	1.00	24.25
		ATOM	1954	N	ILE .	A 281	73.462	59.668	25.460	1.00	24.22
		ATOM	1955	CA	ILE .	A 281	74.349	60.044	24.346	1.00	26.13
		ATOM	1956	CB	ILE .	A 281	74.150	61.514	23.913	1.00	25.19
		ATOM	1957	CG2	ILE	A 281 ·	.75.294	61.981	23.010	1.00	27.25
•	20	MOTA	1958	CG1	ILE	A 281	72.804	61.683	23.216	1.00	24.20
		MOTA	1959	CD1	ILE	A 281	72.269	63.097	23.280	1.00	25.74
		MOTA	1960	C	ILE	A 281	75.817	59.824	24.663	1.00	26.96
		MOTA	1961	0	ILE	A 281	76.585	59.418	23.783	1.00	24.09
	•	MOTA	1962	N	ARG	A 282	76.220	60.108	25.915	1.00	26.63
	25	MOTA	1963	CA	ARG	A 282	77.614	59.937	26.315	1.00	26.66
		MOTA	1964	CB	ARG	A 282	77.883	60.575	27.693	1.00	30.42
		ATOM	1965	CG	ARG	A 282	79.344	60.496	28.132	1.00	33.94
		ATOM	1966	CD	ARG	A 282	79.574	61.182	29.482	1.00	38.66
		MOTA	1967	NE	ARG	Á 282	80.944	60.996	29.981	1.00	41.54
	.30	MOTA	1968	CZ	ARG	A 282	82.028	61.599	29.469	1.00	44.32
		ATOM	1969	NH1	ARG	A 282	81.928	62.399	28.406	1.00	46.32
		MOTA	1970	NH2	ARG	A 282	83.220	61.401	30.023	1.00	45.03
		MOTA	1971	C	ARG	A 282	77.986	58.457	26.321	1.00	24.24
		MOTA	1972	0	ARG	A 282	79.117	58.089	26.016	1.00	23.52
	35	ATOM	1973	N	GLU	A 283	77.023	57.614	26.637	1.00	23.65

	MOTA	1974	CA	GLU Z	Ą	283	77.246	56.170	26.645	1.00	25.88
	ATOM	1975	CB	GLU Z	Ą	283	76.023	55.468	27.224	1.00	25.65
	MOTA	1976	CG	GLU Z	A	283	75.594	55.991	28.587	1.00	32.93
	MOTA	1977	CD	GLU I	A	283	76.041	55.084 .	29.709	1.00	33.42
5	MOTA	1978	OE1	GLU 1	A	283	75.163	54.544	30.412	1.00	35.74
	MOTA	1979	OE2	GLU Z	A	283	77.268	54.899	29.871	1.00	34.68
	MOTA	1980	С	GLU Z	A	283	77.519	55.632	25.219	1.00	26.49
	MOTA	1981	0	GLU I	A	283	78.075	54.556	25.056	1.00	26.00
	MOTA	1982	И.	MET 2	A	284	77.106	56.387	24.195	1.00	28.65
10	ATOM	1983	CA	MET .	A	284	77.292	55.981	22.790	1.00	30.37
	MOTA	1984	СВ	MET .	A	284	76.193	56.578	21.907	1.00	29.17
	ATOM	1985	CG ·	MET .	Ą	284	74.799	56.484	22.496	1.00	28.48
	MOTA	1986	SD	MET .	A	284	73.490	56.940	21.341	1.00	32.72
	ATOM	1987	CE	MET	A	284	73.068	58.578	21.912	1.00	30.81
15	ATOM	1988	С	MET	A	284	78.662	56.353	22.236	1.00	31.62
·	ATOM	1989	0	MET	A	284	78.971	55.995	21.110	1.00	32.97
•	ATOM	1990	N	ASN	A	285	79.483	57.082	23.016	1.00	33.38
	ATOM	1991	CA	ASN	A	285	80.818	57.508	22.563	1.00	35.76
	MOTA	1992	CB	ASN	A	285	81.777	56.317	22.434	1.00	35.36
20	ATOM	1993	CG	ASN	A	285	81.930	55.498	23.708	1.00	37.66
	MOTA	1994	OD1	ASN	A	285	82.275	54.311	23.659	1.00	35.39
•	MOTA	1995	ND2	ASN	A	285	81.678	56.123	24.853	1.00	36.16
	MOTA	1996	C	ASN	A	285	80.707	58.241	21.204	1.00	37.50
	MOTA	1997	0	ASN	A	285	81.275	57.809	20.198	1.00	37.75
25	ATOM .	1998	N	PRO	A	286	79.964	59.351	21.170	1.00	38:06
	ATOM	1999	CD	PRO	A	286	79.255	59.943	22.329	1.00	37.89
	MOTA	2000	CA	PRO	A	286	79.750	60.131	19.947	1.00	39.95
	ATOM	2001	CB	PRO	A	286	78.659	61.121	20.362	1.00	39.05
	MOTA	2002	CG	PRO	A	286	78.886	61.302	21.826	1.00	38.06
30	MOTA	2003	С	PRO	A	286	80.974	60.911	19.486	1.00	40.66
	MOTA	2004	0	PRO	A	286	81.759	61.425	20.291	1.00	40.65
•	MOTA	2005	Ŋ	ASN	A	287	81.103	61.051	18.171	1.00	41.08
	MOTA	2006	CA	ASN	A	287	82.194	61.830	17.633	1.00	41.25
	MOTA	2007	CB	ASN	A	287	82.902	61.108	16.493	1.00	43.10
35	MOTA	2008	CG	ASN	A	. 287	84.105	60.323	16.998	1.00	4.2.68

	MOTA	2009	OD1	ASN	A	287		84.162	59.101	16.876	1.00	42.74
	ATOM	2010	ND2	ASN	A	287		85.074	61.027	17.573	1.00	42.61
	MOTA	2011	С	ASN	A	287		81.687	63.222	17.269	1.00	40.62
	ATOM	2012	0	ASN	A	287		82.456	64.141 .	17.021	1.00	40.65
5	MOTA	2013	N	TYR	A	288		80.367	63.359	17.310	1.00	41.10
	ATOM	2014	CA	TYR	A	288		79.658	64.611	17.060	1.00	42.21
	ATOM	2015	CB	TYR	A	288		79.602	65.014	15.569	1.00	42.33
	MOTA	2016	CG .	TYR	A	288		79.418	63.880	14.588	1.00	42.43
•	MOTA	2017	CD1	TYR	A	288		80.507	63.341	13.914	1.00	42.88
10	MOTA	2018	CE1	TYR	A	288		80.351	62.306	13.006	1.00	42.57
	MOTA	2019	CD2	TYR	A	288		78.159	63.354	14.326	1.00	43.59
	ATOM	2020	CE2	TYR	A	288		77.993	62.319	13.420	1.00	42.81
	MOTA	2021	CZ	TYR	A	288		79.093	61.798	12.765	1.00	42.73
	MOTA	2022	ОН	TYR	A	288		78.934	60.750	11.876	1.00	43.10
15	ATOM	2023	С	TÝR	A	288		78.262	64.512	17.645	1.00	43.00
	MOTA	2024	0	TYR	A	288		77.644	63.450	17.612	1.00	40.24
	MOTA	2025	N	THR	A	289		77.776	65.611	18.203	1.00	44.37
	MOTA	2026	CA	THR	A	289		76.451	65.614	18.812	1.00	47.10
	MOTA	2027	CB	THR	A	289		76.541	65.473	20.347	1.00	46.92
20	MOTA	2028	OG1	THR	A	289		76.811	66.725	20.970	1.00	45.80
	MOTA	2029	CG2	THR	A	289		77.581	64.474	20.816	1.00	45.35
	ATOM	2030	С	THR	A	289		75.666	66.861	18.435	1.00	48.71
	ATOM	2031	0	THR	A	289		74.506	66.994	18.816	1.00	49.12
	MOTA	2032	N	GLU	A	290	•	76.307	67.767	17.687	1.00	50.41
25	ATOM	2033	CA	GLU	A	290		75.674	69.008	17.251	1.00	52.56
	ATOM	2034	CB	GLU	A	290		76.706	69.963	16.653	1.00	54.21
	ATOM	2035	CG	GLU	A	290		77.852	70.307	17.595	1.00	56.44
	MOTA	2036	CD	GLU	A	290		79.112	69.509	17.307	1.00	58.31
	MOTA	2037	OE1	GLU	A	. 290		80.205	70.115	17.278	1.00	59.38
30	ATOM	2038	OE2	GLU	A	290		79.009	68.278	17.113	1.00	58.91
	MOTA	2039	C	GLU	A	290		74.556	68.733	16.251	1.00	53.63
	MOTA	2040	0	GLU	A	290		74.504	69.325	15.176	1.00	53.39
	ATOM	2041	N	PHE	P	291		73.665	67.829	16.627	1.00	54.78
	ATOM	2042	CA	PHE	7	291		72.535	67.445	15.809	1.00	56.14
35	MOTA	2043	CB	PHE	P	291		72.090	66.025	16.169	1.00	56.00

	ATOM	2044	CG	PHE A	291	72.958	64.947	15.603	1.00	56.83
	ATOM	2045	CD1	PHE A	291	73.985	64.405	16.353	1.00	56.77
	ATOM	2046	CD2	PHE A	291 .	72.740	64.467	14.321	1.00	57.19
	ATOM	2047	CE1	PHE A	291	74.781	63.401 .	15.836	1.00	57.29
5	ATOM	2048	CE2	PHE A	291	73.533	63:464	13.799	1.00	57.70
	ATOM	2049	CZ	PHE A	291	74.556	62,930	14.558	1.00	57.44
	ATOM	2050	С	PHE A	291 ·	71.376	68.409	16.018	1.00	57.37
	ATOM	2051	0	PHE A	291	71.563	69.557	16.413	1.00	58.88
	MOTA	2052	N	LYS A	292	70.180	67.931	15.748	1.00	57.76
10	ATOM .	2053	CA	LYS A	292	68.979	68.726	15.893	1.00	58.17
	ATOM .	2054	CB	LYS A	292	68.738	69.566	14.628	1.00	60.13
	ATOM	2055	CG	LYS A	292	69.554	69.120	13.402	1.00	61.32
	ATOM	2056	CD	LYS A	292	69.445	67.616	13.137	1.00	61.28
	ATOM	2057	CE	LYS A	292	68.585	67.313	11.926	1.00	61.42
15	ATOM	2058	NZ	LYS A	292	67.875	66.014	12.071	1.00	62.17
	ATOM	2059	С	LYS A	292	67.804	67.798	16.171	1.00	57.78
	ATOM	2060	0	LYS A	292	67.150	67.291	15.252	1.00	58.28
	ATOM	2061	N	PHE A	293	67.575	67.541	17.451	1.00	56.83
	MOTA	2062	CA	PHE A	293	66.516	66.640	17.871	1.00	55.06
20	ATOM	2063	CB	PHE A	293	66.832	66.024	19.244	1.00	54.49
	ATOM	2064	CG	PHE A	293	68.277	65.646	19.440	1.00	52.66
	ATOM	2065	CD1	PHE A	293	68.885	64.716	18.615	1.00	52.89
	MOTA	2066	CD2	PHE A	293	69.026	66.224	20.454	1.00	51.93
	ATOM ·	2067	ÇE1	PHE A	293	70.213	64.368	18.795	1.00	52.57
25	ATOM	2068	CE2	PHE A	293	70.354	65.883	20.641	1.00	52.26
	ATOM	2069	CZ	PHE A	293	70.949	64.952	19.809	1.00	52.07
	ATOM	2070	C	PHE A	293	65.165	67.340	17.888	1.00	54.04
	ATOM	2071	0	PHE A	293	65.037	68.457	18.391	1.00	53.67
	MOTA	2072	N	PRO A	294	64.136	66.688	17.317	1.00	53.78
30	ATOM	2073	CD	PRO A	294	64.223	65.365	16.670	1.00	53.01
	ATOM	2074	CA	PRO A	294 ·	62.779	67.248	17.254	1.00	53.38
	MOTA	2075	CB	PRO A	294	62.006	66.233	16.401	1.00	53.26
	MOTA	2076	CG	PRO A	294	62.786	64.967	16.496	1.00	53.31
	ATOM	2077	С	PRO A	294	62.117	67.413	18.635	1.00	52.79
35	MOTA	2078	0	PRO A	294	61.031	67.995	18.742	1.00	53.69

	MOTA	2079	N	GLN A 295	62.766	66.901	19.684	1.00 51.09
	ATOM	2080	CA	GLN A 295	62.235	66.989	21.053	1.00 49.40
	ATOM	2081	CB	GLN A 295	62.135	68.440	21.532	1.00 47.56
	ATOM	2082	CG	GLN A 295	63.474	69.148 .	21.658	1.00 46.71
5	ATOM	2083	CD	GLN A 295	64.518	68.322	22.382	1.00 45.57
	ATOM	2084	OE1	GLN A 295	64.234	67.695	23.393	1.00 45.44
	MOTA	2085	NE2	GLN A 295	65.737	68.324	21.868	1.00 45.50
	ATOM	2086	С	GLN A 295	60.888	66.285	21.173	1.00 48.71
	ATOM	2087	0	GLN A 295	59.828	66.920	21.166	1.00 48.11
10	ATOM	2088	N	IĻE A 296	60.944	64.961	21.274	1.00 47.95
•	ATOM	2089	CA	ILE A 296	59.745	64.145	21.384	1.00 47.97
	MOTA	2090	CB	ILE A 296	59.590	63.210	20.160	1.00 47.45
	MOTA	2091	CG2	ILE A 296	58.156	62.723	20.041	1.00 47.21
	MOTA	2092	CG1	ILE A 296	60.015	63.927	18.873	1.00 47.88
15	ATOM	2093	CD1	ILE A 296	60.015	63.036	17.649	1.00 48.40
	ATOM	2094	С	ILE A 296	59.765	63.295	22.652	1.00 47.76
	ATOM	2095	0	ILE A 296	60.830	63.005	23.208	1.00 48.33
	ATOM	2096	N	LYS A 297	58.579	62.877	23.084	1.00 47.32
	MOTA	2097	CA	LYS A 297	58.441	62.032	24.264	1.00 46.79
20	MOTA	2098	СВ	LYS A 297	57.278	62.505	25.171	1.00 48.16
	MOTA	2099	CG	LYS A 297	56.17.4	63.305	24.466	1.00 48.76
	MOTA	2100	CD	LYS A 297	56.550	64.778	24.251	1.00 50.38
	ATOM	2101	CE	LYS A 297	56.720	65.542	25.569	1.00 50.43
•	MOTA	2102	NZ	LYS A 297	57.428	66.847	25.376	1.00 49.71
25	MOTA	2103	C	LYS A 297	58.234	60.584	23.819	1.00 46.40
	MOTA	2104	0	LYS A 297	57.437	60.318	22.917	1.00 46.93
	MOTA	2105	N	ALA A 298	58.980	59.659	24.427	1.00 45.46
	ATOM	2106	CA	ALA A 298	58.911	58.237	24.079	1.00 45.16
	MOTA	2107	СВ	ALA A 298	59.583	57.377	25.139	
30	MOTA	2108	С	ALA A 298	57.494	57.744	23.819	•
	MOTA	2109	0	ALA A 298	56.558	58.075		<u></u>
	MOTA	2110	N	HIS A 299	57.357	56.923	22.782	
	MOTA	2111	. CA	HIS A 299	56.075			
	MOTA	2112	2 CE	B HIS A 299	55.975			
35	MOTA	2113	3 CG	HIS A 299	54.587	55.926	20.361	1.00 43.08

	ATOM	2114	CD2	HIS	A	299	54.047	54.824	19.788	1.00	43.51
	MOTA	2115	ND1	HIS	A	299	53.574	56.864	20.399	1.00	43.83
	ATOM	2116	CE1	HIS	A	299	52.474	56.351	19.878	1.00	43.22
	MOTA	2117	NE2	HIS	A	299	52.734	55.113	19.499	1.00	42.58
5	ATOM	2118	C	HIS	A	299	55.959	54.963	23.078	1.00	44.10
	MOTA	2119	0	HIS	A	299	56.782	54.080	22.838	1.00	44.94
	ATOM	2120	N	PRO	A	300	54.944	54.769	23.936	1.00	43.53
	ATOM	2121	CD	PRO	A	300	53.921	55.772	24.283	1.00	43.05
	ATOM	2122	CA	PRO	A	300	54.737	53.501	24.649	1.00	42.90
10	ATOM	2123	CB	PRO	A	300	53.286	53.614	25.116	1.00	43.38
	ATOM	2124	CG	PRO	A	300 .	53.090	55.076	25.330	1.00	43.66
	ATOM	2125	C	PRO	A	300	54.911	52.287	23.741	1.00	42.52
	ATOM	2126	0	PRO	A	300	54.217	52.152	22.735	1.00	42.26
	MOTA	2127	N	TRP	A	301	55.846	51.410	24.103	1.00	42.18
15 ·	ATOM	2128	CA	TRP	A	301	56.120	50.207	23.322	1.00	42.14
•	ATOM	2129	CB	TRP	A	301	57.165	49.330	24.015	1.00	41.33
	MOTA	2130	CG	TRP	A	301	58.583	49.696	23.682	1.00	40.34
	MOTA	2131	CD2	TRP	A	301	59.190	49.696	22.380	1.00	39.60
	ATOM	2132	CE2	TRP	A	301	60.527	50.110	22.543	1.00	39.49
_20	ATOM	2133	CE3	TRP	A	301	58.731	49.387	21.095	1.00	39.48
	ATOM	2134	CD1	TRP	A	301	59.556	50.098	24.556	1.00	40.21
	ATOM	2135	NE1	TRP	A	301	60.726	50.351	23.879	1.00	39.18
	MOTA	2136	CZ2	TRP	A	301 .	61.407	50.220	21.470	1.00	39.55
	MOTA	2137	CZ3	TRP	A	301	59.604	49.497	20.033	1.00	38.40
25	ATOM	2138	CH2	TRP	A	301	60.925	49.910	20.224	1.00	39.52
	ATOM	2139	С	TRP	A	301	54.852	49.407	23.052	1.00	43.11
	ATOM	2140	0	TRP	A	301	54.690	48.830	21.975	1.00	43.94
	ATOM	2141	N	THR	A	302	53.953	49.375	24.032	1.00	44.41
	MOTA	2142	CA	THR	A	302	52.692	48.643	23.901	1.00	45.14
30	MOTA	2143	CB	THR	A	302	51.997	48.489	25.259	1.00	45.40
	MOTA	2144	OG1	THR	A	302	50.806	47.733	25.138	1.00	47.13
	MOTA	2145	CG2	THR	A	302	51.662	49.797	25.943	1.00	45.17
	ATOM	2146	C	THR	A	302	51.763	49.282	22.860	1.00	45.41
,	MOTA	2147	0	THR	A	302	50.902	48.608	22.286	1.00	46.19
35	ATOM	2148	N	LYS	A	303	51.964	50.573	22.599	1.00	44.91

	ATOM	2149	CA	LYS A	303	51.172	51.295 .	21.607	1.00	44.23
	ATOM	2150	СВ	LYS A	303	50.962	52.747	22.053	1.00	45.50
	MOTA	2151	CG	LYS A	303	49.656	52.991	22.792	1.00	47.39
	ATOM	2152	CD	LYS A	303	49.381	54.483 .	22.937	1.00	49.70
5 *	MOTA	2153	CE	LYS A	303	48.426	54.994	21.863	1.00	50.84
	ATOM	2154	NZ	LYS A	303	47.185	55.585	22.445	1.00	51.69
	ATOM	2155	C ·	LYS A	303	51.862	51.272	20.227	1.00	43.47.
•	ATOM	2156	0	LYS A	303	51.232	51.562	19.212	1.00	42.78
	ATOM	2157	N	VAL A	304	53.158	50.936	20.199	1.00	42.34
10	ATOM	2158	CA	VAL A	304	53.917	50.891	18.943	1.00	42.40
	ATOM	2159	CB	VAL A	304	55.442	50.779	19.184	1.00	42.11
	ATOM	2160	CG1	VAL A	304	56.177	50.320	17.921	1.00	40.82
	MOTA	2161	CG2	VAL A	304	56.002	52.102	19.681	1.00	39.70
	MOTA	2162	С	VAL A	304	53.450	49.748	18.042	1.00	42.22
15	MOTA	2163	0	VAL A	304	53.406	49.890	16.821	1.00	43.06
	MOTA	2164	N	PHE A	305	53.106	48.617	18.652	1.00	41.61
	MOTA	2165	CA	PHE A	305	52.649	47.452	17.906	1.00	41.24
•	MOTA	2166	CB	PHE A	305	53.269	46.176	18.472	1.00	37.57
	MOTA	2167	CG	PHE A	305	54.763	46.198	18.469	1.00	35.03
20	ATOM	2168	CD1	PHE A	305	55.463	46.597	19.598	1.00	33.16
	MOTA	2169	CD2	PHE A	305	55.470	45.834	17.335	1.00	33.57
	ATOM	2170	CE1	PHE A	305	56.838	46.632	19.597	1.00	31.36
	ATOM	2171	CE2	PHE A	305	56.850	45.865	17.328	1.00	32.96
	ATOM	2172	CZ	PHE A	. 305	57.534	46.265	18.462	1.00	33.78
25	MOTA	2173	С	PHE A	305	51.135	47.345	17.901	1.00	42.81
	MOTA	2174	0	PHE A	305	50.455	47.939	18.738	1.00	44.77
	MOTA	2175	N	ARG A	306	50.606	46.579	16.955	1.00	44.27
	MOTA	2176	CA	ARG A	306	49.169	46.398	16.859	1.00	45.78
	MOTA	2177	CB	ARG A	306	48.788	45.720	15.541	1.00	47.80
30	MOTA	2178	CG	ARG A	A 306	49.444	44.366	15.315	1.00	50.54
	MOTA	2179	CD	ARG A	A 306	49.697	44.111	13.829	1.00	52,93
	MOTA	2180	NE	ARG A	A 306	48.876	43.013	13.315	1.00	55.30
	MOTA	2181	CZ	ARG A	A 306	49.028	41.731	13.669	1.00	56.25
	ATOM	2182	NHI	ARG I	A :306	49.967	41.375	14.547	1.00	55.27
35	MOTA	2183	NH2	2 ARG A	A: 306	48.233	40.801	13.143	1.00	56.50

	MOTA	2184	С	ARG	A	306	48.663	45.589	18.049	1.00	45.74
	ATOM	2185	0	ARG	A	30 <u>6</u>	49.404	44.793	18.619	1.00	45.14
	MOTA	2186	N	PRO	A	307	47.397	45.793	18.453	1.00	46.23
	MOTA	2187	CD	PRO	A	307	46.442	46.735 .	17.846	1.00	46.07
5	ATOM	2188	CA	PRO	A	307	46.811	45.082	19.592	1.00	46.18
	MOTA	2189	СВ	PRO	A	307	45.340	45.530	19.597	1.00	46.66
	MOTA	2190	CG	PRO	A	307	45.115	46.175	18.269	1.00	46.15
	ATOM	2191	С	PRO	A	307	46.909	43.567	19.444	1.00	46.73
	MOTA	2192	0	PRO	A	307	47.062	43.049	18.339	1.00	47.71
10	ATOM	2193	N .	ARG	A	308	46.820	42.870	20.574	1.00	46.74
	MOTA	2194	CA	ARG	A	308 .	46.889	41.411	20.605	1.00	46.91
	MOTA	2195	CB	ARG	A	308	45.830	40.797	19.674	1.00	49.70
	MOTA	2196	CG	ARG	A	308	44.566	40.340	20.406	1.00	52.99
	MOTA	2197	CD	ARG	A	308	44.655	38.885	20.869	1.00	57.02
15	MOTA	2198	NE	ARG	A	308	45.943	38.578	21.513	1.00	60.77
	ATOM .	2199	CZ	ARG	A	308	46.106	38.320	22.825	1.00	61.29
	MOTA	2200	NH1	ARG	A	308	45.061	38.310	23.659	1.00	61.76
	ATOM	2201	NH2	ARG	A	308	47.326	38.070	23.300	1.00	61.20
	ATOM	2202	Ç	ARG	A	308	48.292	40.881	20.274	1.00	44.79
20 .	MOTA	2203	0	ARG	A	308	48.471	39.680	20.055	1.00	43.82
	MOTA	2204	N	THR	A	309	49.294	41.760	20.285	1.00	42.99
	ATOM	2205	CA	THR	A	309	50.675	41.332	20.030	1.00	41.54
	ATOM ·	2206	CB	THR	A	309	51.547	42.495	19.525	1.00	39.98
	ATOM ·	2207	OG1	THR	A	309	51.117	42.936	18.253	1.00	39.67
25	MOTA	2208	CG2	THR	A	309	53.022	42.166	19.418	1.00	38.09
	MOTA	2209	C	THR	A	309	51.258	40.740	21.315	1.00	40.62
	MOTA	2210	0	THR	A	309	51.132	41.336	22.382	1.00	41.53
•	MOTA	2211	N	PRO	A	310	51.883	39.551	21.238	1.00	39.36
	ATOM	2212	CD	PRO	A	310	52.065	38.755	20.008	1.00	38.76
30	ATOM	2213	CA	PRO	A	310	52.461	38.881	22.415	1.00	38.43
	ATOM	2214	CB	PRO	A	310	53.390	37.843	21.792	1.00	37.91
	ATOM	2215	CG	PRO	A	310	52727	37.494	20.500	1.00	39.30
	ATOM	2216	C.	PRO	A	310	53.247	39.846	23.309	1.00	36.53
·	ATOM	2217	0	PRO	A	310	54.293	40.349	22.918	1.00	37.72
35	ATOM	2218	N	PRO	A	311	52.744	40.113	24.530	1.00	34.81

	ATOM	2219	CD	PRO A	311	51.498	39.546	25.078	1.00	34.82
	ATOM	2220	CA	PRO A	311	53.400	41021	25.487	1.00	32.04
	ATOM	2221	CB	PRO A	311	52.619	40.791	26.779	1.00	33.08
	ATOM	2222	CG	PRO A	311	51.272	40.357 .	26.321	1.00	35.07
5	MOTA	2223 .	C	PRO A	311	54.878	40.685	25.682	1.00	29.08
	ATOM	2224	0	PRO A	311	55.706	41.577	25.833	1.00	28.54
	ATOM	2225	N	GLU A	312	55.202	39.396	25.647	1.00	28.12
	ATOM	2226	CA	GLU A	312	56.578	38.937	25.791	1.00	28.15
	ATOM	2227	СВ	GLU A	312	56.624	37.416	25.989	1.00	32 438
10	ATOM	2228	CG	GLU A	312	55.811	36.917	27.186	1.00	38.17
	ATOM	2229	CD	GLU A	312	54.382	36.502	26.839	1.00	40.82
	ATOM	2230	OE1	GLU A	312 .	53.864	35:572	27.490	1.00	43.31
	ATOM	2231	OE2	GLU A	312	53.775	37.105	25.923	1.00	42.33
	MOTA	2232	С	GLU A	312	57.434	39.373	24.586	1.00	26.26
15	MOTA	2233	0	GLU A	312	58.625	39.636	24.729	1.00	25.86
	ATOM	2234	N	ALA A	313	56.805	39.489	23.407	1.00	24.44
	MOTA	2235	CA	ALA A	313	57.502	39.945	22.188	1.00	24.09
	MOTA	2236	CB	ALA A	313 .	56.615	39.725	20.955	1.00	22.36
	MOTA	2237	С	ALA A	313	57.835	41.425	22.332.	1.00	22.39
20	ATOM	2238	0	ALA A	313	58.938	41.864	22.034	1.00	23.16
	ATOM	2239	N	ILE A	314	56,871	42.183	22.835	1.00	22.65
	ATOM	2240	CA .	ILE A	314	57.047	43.610	23.076	1.00	23.93
	ATOM	2241	CB.	ILE A	314	55.708	44.254	23.514	1.00	24.11
	ATOM	2242	CG2	ILE A	314	55.833	45.766	23.637	1.00	27.02
25	ATOM	2243	CG1	ILE A	314	54.597	43.894	22.527	1.00	25.37
	MOTA	2244	CD1	ILE A	314	53.285	44.616	22.774	1.00	23.59
	MOTA	2245	С	ILE A	314	58.118	43.841	24.149	1.00	23.96
	ATOM	2246	0	ILE A	. 314	58.948	44.748	24.043	1.00	25.44
	MOTA	2247	N.	ALA A	315	58.114	43.002	25.190	1.00	24.48
30	MOTA	2248	CA	ALA A	315	59.101	43.127	26.275	1.00	21.38
	ATOM	2249	CB	ALA A	315	58.794	42.130	27.378	1.00	18.99
	MOTA	2250	С	ALA A	315	60.525	42.939	25.753	1.00	20.50
	MOTA	2251	0	ALA A	315	61.425	43.723	26.078	1.00	18.67
	ATOM	2252	N	LEU A	316	60.725	41.892	24.928	1.00	19.20
35	ATOM	2253	CA	LEU A	316	62.045	41.609	24.344	1.00	19.31

	ATOM	2254	СВ	LEU A	£	316	62.010	40.265	23.565	1.00	19.88
	ATOM	2255	CG	LEU A	Ą	316	63.240	39.902	22.709	1.00	17.67
	ATOM	2256	CD1	LEU Z	A	316	64.464	39.652	23.567	1.00	15.53
	ATOM	2257	CD2	LEU Z	A	316	62.956	38.685 .	21.848	1.00	17.95
5	ATOM	2258	С	LEU 2	A	316	62.510	42.792	23.466	1.00	18.37
	ATOM	2259	0	LEU A	Ą	316	63.686	43.175	23.480	1.00	18.43
	ATOM	2260	N	CYS A	ď	317	61.566	43.396	22.739	1.00	18.93
	MOTA	2261	CA	CYS A	Ą	317	61.852	44.557	21.884	1.00	22.24
	ATOM	2262	CB	CYS I	Ą	317	60.592	44.975	21.114	1.00	25.99
10	ATOM	2263	SG	CYS A	Ą	317	60.621	44.562	19.353	1.00	36.98
	ATOM	2264	С	CYS Z	Ą	317	62.384	45.751	22.681	1.00	22.08
•	ATOM	2265	0	CYS 2	Ą	317	63.337	46.422	22.253	1.00	18.81
	ATOM	2266	N	SER 2	A	318	61.761	46.029	23.849	1.00	21.02
	MOTA	2267	CA	SER A	A	318	62.199	47.159	24.695	1.00	19.59
15	ATOM	2268	CB	SER 2	Ą	318	61.212	47.439	25.856	1.00	23.13
	MOTA	2269	OG	SER 3	A	318	60.959	46.274	26.641	1.00	19.46
	MOTA	2270	C	SER 2	A	318	63.621	46.960	25.222	1.00	18.44
	ATOM	2271	0	SER I	A	318	64.365	47.920	25.386	1.00	18.50
	ATOM	2272	Ń	ARG .	A	319	64.001	45.708	25.480	1.00	19.95
20	MOTA	2273	CA	ARG .	A	319	65.337	45.401	25.997	1.00	21.38
	MOTA	2274	CB	ARG .	A	319	65.293	44.140	26.861	1.00	23.27
	ATOM	2275	CG	ARG .	A	319	64.261	44.200	27.983	1.00	25.35
	ATOM	2276	CD.	ARG .	A	319	64'.580	45.302	28.979	1.00	23.98
	ATOM	2277	NE	ARG .	A	319	65.984	45.280	29.403	1.00	28.61
25	ATOM	2278	CZ	ARG	A	319	66.559	44.274	30.092	1.00	27.11
	ATOM	2279	NH1	ARG	A	319	65.851	43.219	30.478	1.00	27.95
	ATOM	2280	NH2	ARG	A	319	67.849	44.335	30.397	1.00	28.62
	ATOM	2281	С	ARG	A	319	66.403	45.239	24.899	1.00	22.00
	ATOM	2282	0	ARG	A	319	67.574	45.011	25.217	1.00	21.44
30	MOTA	2283	N	LEU	A	320	66.001	45.364	23.620	1.00	20.51
	ATOM	2284	CA	LEU	A	320	66.947	45.248	22.481	1.00	18.20
	ATOM	2285	CB	LEU	A	320	66.417	44.282	21.390	1.00	15.82
	ATOM	2286	CG	LEU	A	320	66.077	42.864	21.851	1.00	13.56
	ATOM	228.7	CD1	LEU	A	320	65.158	42.168	20.860	1.00	12.01
35	ATOM	2288	CD2	LEU	A	320	67.332	42.048	22.104	1.00	14.30

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	MOTA	2289	C	LEU A	7	320	67.167	46.613	21.886	1.00	14.55
	MOTA	22,90	0	LEU A	7	320	68.285	47.015	21.649	1.00	17.73
	MOTA	2291	N	LEU F	7	321	66.074	47.332	21.680	1.00	15.67
	ATOM	·2292	CA	LEU F	7	321	66.126	48.680	21.144	1.00	17.61
- 5	ATOM	2293	CB	LEU	Ā	321	64.892	48.978	20.278	1.00	15.07
	MOTA	2294	CG	LEU F	7	321	64.632	47.982	19.146	1.00	17.45
	ATOM	2295	CD1	LEU A	Į	321	63.217	48:144	18.622	1.00	12.07
	MOTA	2296	CD2	LEU F	Ą	321	65.674	48.164	18.038	1.00	11.94
	ATOM	2297	C	LEU F	Ą	321	66.266	49.730	22.255	1.00	17.32
10	ATOM	2298	0	LEU A	j	321	65.358	50.514	22.500	1.00	15.83
	ATOM	2299	N	GLU A	7	322	67.424	49.746	22.897 .	1.00	20.87
	ATOM	2300	CA	GLU A	Ĵ	322	67.708	50.697	23.970	1.00	21.68
	MOTA	2301	CB	GLU A	Ą	322	68.114	49.931	25.246	1.00	22.81
	MOTA	2302	· CG	GLU A	Ą	322	67.688	50.614	26.542	1.00	28.40
15	MOTA	2303	CD	GLU A	Ą	322	66.652	49.815	27.315	1.00	28.36
	MOTA	2304	OE1	GLU Z	A	322	66.875	48.605	27.546	1.00	30.00
	MOTA	2305	OE2	GLU Z	A	322	65.613	50.399	27.684	1.00	30.22
	MOTA	2306	С	GLU I	Ą	322	68.826	51.605	23.553	1.00	19.57
	MOTA	2307	. 0	GLU I	A	322	69.808	51.136	22.986	1.00	24.35
20	MOTA	2308	N	TYR A	A	323	68.682	52.901	23.824	1.00	19.26
	ATOM	2309	CA	TYR A	A	323	69.698	53.893	23.464	1.00	19.31
	MOTA	2310	CB	TYR	A	323 -	69.282	55.295	23.925	1.00	22.25
	ATOM	2311	CG	TYR .	A	323	68.382	56.044	22.971	1.00	22.48
	MOTA	2312	CD1	TYR	A	323	68.689	56.162	21.610	1.00	22.04
25	MOTA	2313	CE1	TYR .	A	323	67.847	56.859	20.750	1.00	21.95
	MOTA	2314	CD2	TYR	A	323	67.226	56.643	23.434	1.00	21.41
	MOTA	2315	CE2	TYR	A	323	66.386	57.337	22.587	1.00	24.39
	MOTA	2316	CZ	TYR	A	323	66.698	57.442	21.244	1.00	23.89
	MOTA .	2317	ОН	TYR	A	323	65.849	58.133	20.405	1.00	23.70
30	ATOM	2318	С	TYR	A	323	71.074	53.553	24.030	1.00	19.93
	MOTA	2319	0	TYR	A	323	72.083	53.580	23.304	1.00	17.86
	ATOM	2320	N	THR	A	324	71.127	53.228	25.339	1.00	19.13
	MOTA	2321	CA	THR	A	324	72.401	52.875	25.971	1.00	15.51
	ATOM	2322	CB	THR	A	324	72.339	52.986	27.507	1.00	17.08
35	MOTA	2323	OG1	THR	A	324	71.807	54.245	27.879	1.00	17.91

	MOTA	2324	CG2	THR A	324	73.699	52.853	28.147	1.00 1	1.22
	ATOM	2325	С	THR A	324	72.800	51.489	25.541	1.00 1	4.29
	ATOM	2326	0	THR A	324	72.045	50.542	25.741	1.00 1	4.20
	ATOM	2327	N	PRO A	. 325 ·	73.977	51.373 .	24.886	1.00 1	6.36
5	ATOM	2328	CD	PRO A	325	74.882	52.494°	24.586	1.00 1	4.52
	ATOM	2329	CA	PRO A	325	74.486	50.099	24.329	1.00 1	4.39
	ATOM•	2330	CB	PRO A	325	75.848	50.481	23.743	1.00 1	0.98
	ATOM	2331	CG	PRO A	325	75.763	51.937	23.498	1.00 1	5.41
	ATOM	2332	С	PRO A	325	74.636	48.983	25.365	1.00 1	5.34
10	ATOM	2333	0	PRO A	325	74.214	47.840	25.130	1.00 1	2.17
•	ATOM	2334	N .	THR A	326	75.237	49.323	26.514	i.00 1	5.65
	MOTA	2335	CA	THR A	326	75.435	48.354	27.610 ·	1.00 1	4.91
	MOTA	2336	CB	THR A	326	76.305	48.965	28.718	1.00 1	4.59
•	MOTA	2337	OG1	THR A	326	75.804	50.224	29.130	1.00 1	1.75
15	MOTA	2338	CG2	THR A	326	77.744	49.150	28.302	1.00 1	3.98
	ATOM	2339	C	THR F	326	74.119	47.875	28.196	1.00 1	4.19
	ATOM	2340	0	THR P	326	74.060	46.813	28.802	1.00 1	9.56
•	ATOM	2341	N	ALA A	327	73.072	48.668	28.024	1.00 1	4.86
	ATOM	2342	CA	ALA A	A 327	71.744	48.358	28.542	1.00 1	5.10
20	ATOM	2343	СВ	ALA A	A 327	70.915	49.624	28.593	1.00 1	5.94
•	MOTA	2344	С	ALA A	A 327	70.989	47.256	27.763	1.00 1	7.36
	ATOM	2345	0	ALA A	A 327	70.043	46.643	28.303	1.00 1	5.08
	MOTA	2346	N	ARG A	A 328	71.378	47.013	26.496	1.00 1	6.26
	ATOM	2347	CA	ARG A	A 328	70.705	45.993	25.656	1.00 1	3.02
25	MOTA	2348	CB	ARG A	A 328	71.126	46.134	24.161	1.00 1	3.41
	MOTA	2349	CG	ARG A	A 328	70.732	47.450	23.514	1.00 1	4.63
	ATOM	2350	CD	ARG A	A 328	71.583	47.740	22.255	1.00 1	.7.74
	MOTA	2351	NE	ARG A	A 328	71.432	49.141	21.822	1.00 1	4.76
	ATOM	2352	CZ	ARG I	A 328	72.398	49.869	21.296	1.00 1	.0.22
30 `	ATOM	2353	NH1	ARG A	A 328	73.492	49.298	20.858	1.00	9.59
	MOTA	2354	NH2	ARG .	A 328	72.237	51.187	21.166	1.00	8.94
	MOTA	2355	С	ARG .	A 328	71.057	44.586	26.096	1.00	6.14
•	MOTA	2356	0	ARG	A 328	72.166	44.329	26.486	1.00	8.50
	MOTA	2357	N	LEU	A 329	70.133	43.656	25.949	1.00.	8.48
35	MOTA	2358	CA	LEU	A 329	70.462	42.279	26.273	1.00	L1.70

	MOTA	2359	CB	LEU P	A .	329	6	9.274	41.342	26.034	1.00	13.47
	MOTA	2360	CG	LEU P	1	329	. 6	7.968	41.615	26.736	1.00	18.89
	ATOM	2361	CD1	LEU A	Į.	329	6	6.876	40.769	26.102	1.00	18.93
	ATOM	2362	CD2	LEU A	Į	329	. 6	8.087	41.309 .	28.232	1.00	19.20
5	ATOM	2363	С	LEU F	J	329	7	1.541	41.786	25.343 ⁻	1.00	17.58
•	MOTA	2364	0	LEU A	£	329	7	1.701	42.294	24.185	1.00	18.98
	ATOM	2365	N	THR A	Į	330	7	2.224	40.737	25.793	1.00	17.60
	MOTA	2366	CA	THR A	P.	330	7	3.209	40.089	24.989	1.00	19.09
	MOTA	2367	СВ	THR A	P	330	7	4.271	39.413	25.846	1.00	19.08
10	MOTA	2368	OG1	THR A	A	330	7	73.702	38.399	26.639	1.00	20.66
	ATOM .	2369	CG2	THR A	A	330	7	75.081	40.347	26.725	1.00	22.70
	ATOM	2370	Ċ	THR A	Ą	330	1	72.462	39.012	24.187	1.00	18.93
	ATOM	2371	0	THR I	A	330	-	71.310	38.670	24.495	1.00	19.21
	ATOM	2372	N	PRO 2	A	331	-	73.073	38.459	23.155	1.00	17.26
15	MOTA	2373	CD	PRO .	A	331	-	74.417	38.779	22.661	1.00	17.15
	MOTA	2374	CA	PRO	A _.	331	•	72.409	37.423	22.365	1.00	18.01
	MOTA	2375	CB	PRO .	A	331	•	73.426	37.070	21.277	1.00	13.34
	MOTA	2376	CG	PRO	A	331	•	74.381	38.211	21.255	1.00	17.27
	MOTA	2377	С	PRO	A	331	•	72.060	36.207	23.250	1.00	16.55
20	MOTA	2378	0	PRO	A	331	•	70.967	35.670	23.168	1.00	19.08
	ATOM	2379	N	LEU	A	332	,	72.976	35.786	24.112	1.00	18.64
	MOTA	2380	CA	LEU	A	332		72.676	34.640	24.995	1.00	20.57
	MOTA	2381	CB	LEU	A	332		73.895	34.158	25.770	1.00	22.27
	MOTA	2382	CG	LEU	A	332		73.915	32.659	26.052	1.00	24.61
25	ATOM	2383	CD1	LEU	A	332		73.755	31.869	24.756	1.00	26.96
	MOTA	2384	CD2	LEU	A	332		75.192	32.255	26.780	1.00	26.02
	ATOM	2385	С	LEU	A	332		71.494	34.916	25.919	1.00	17.91
	. ATOM	2386	0	LEU	A	332		70.643	34.060	26.085	1.00	21.79
	MOTA	2387	N	GLU	A	333		71.419	36.133	26.470	1.00	17.14
30	MOTA	2388	CÁ	GLU	A	. 333		70.303	36.544	27.335	1.00	17.62
	MOTA	2389	СВ	GLU	A	. 333		70.599	37.889	28.015	1.00	18.45
	ATOM	2390	CG	GLU	A	333		71.668	37.822	29.095	1.00	19.81
	MOTA	2391	CD	GLU	Ą	333	•	72.216	39.180	29.482	1.0	20.30
	MOTA	2392	OE	1 GLU	P	333		73.258	39.216	30.163	1.0	0 25.89
35	MOTA	2393	OE	2 GLU	P	333		71.622	40.211	29.097	1.0	0 22.23

	MOTA	2394	C	GLU A	333	69.017	36.686	26.540	1.00	18.85
•	ATOM	2395	0	GLU A	333	67.924	36.441	27.056	1.00	18.09
	MOTA	2396	N	ALA A	334	69.127	37.084	25.258	1.00	17.85
	MOTA	2397	CA	ALA A	334	67.917	37.214 .	24.449	1.00	16.32
5	MOTA	2398	СВ	ALA A	334	68.221	37.898	23.097	100	23.05
	MOŢA	2399	С	ALA A	334	67.320	35.841	24.233	1.00	13.30
	MOTA	2400	0	ALA A	334	66.112	35.664	24.301	1.00	15.40
	ATOM	2401	N	CYS A	335	68.189	34.868	23.968	1.00	15.76
	ATOM	2402	CA	CYS A	335	67.786	33.476	23.728	1.00	18.48
10	MOTA	2403	CB	CYS A	335	69.035	32.610	23.453	1.00	20.13
	MOTA	2404	SG	CYS A	335	69.650	32.566	21.730	1.00	23.99
	MOTA	2405	С	CYS A	335	67.038	32.884	24.945	1.00	20.44
	MOTA	2406	0	CYS A	335	66.181	32.014	24.790	1.00	20.18
	MOTA	2407	N	ALA A	336	67.407	33.338	26.156	1.00	21.45
15	ATOM	2408	CA	ALA A	336	66.818	32.844	27.412	1.00	22.45
	ATOM	2409	CB	ALA A	336	67.845	32.902	28.554	1.00	24.12
	MOTA	2410	С	ALA A	336	65.546	33.594	27.780	1.00	21.53
	ATOM	2411	0	ALA A	336	64.811	33.174	28.670	1.00	24.07
	ATOM	2412	N	HIS A	337	65.278	34.687	27.078	1.00	20.73
20	AŢOM	2413	CA	HIS A	337 ⁻	64.083	35.488	27.310	1.00	18.65
	ATOM	2414	CB	HIS A	337	64.014	36.651	26.301	1.00	15.94
	ATOM	2415	CG	HIS A	337	62.994	37.711	26.621	1.00	6.72
	MOTA	2416	CD2	HIS A	337	63.128	38.941	27.167	1.00	7.32
	MOTA	2417	ND1	HIS A	337	61.667	37.572	26.348	1.00	6.66
25	ATOM	2418	CE1	HIS A	337	61.015	38.662	26.701	1.00	5.00
	ATOM	2419	NE2	HIS A	337	61.884	39.507	27.202	1.00	5.30
	MOTA	2420	C	HIS A	337	62.827	34.619	27.284	1.00	19.85
	ATOM	2421	0	HIS A	337	62.839	33.507	26.758	1.00	22.24
	ATOM	2422	N	SER A	338	61.756	35.104	27.886	1.00	19.23
30	ATOM	2423	CA	SER A	338	60.510	34.350	27.961	1.00	21.39
	MOTA	2424	CB	SER A	338	59.595	34.938	29.048	1.00	21.54
	MOTA	2425	OG	SER A	338	58.610	35.797	28.503	1.00	26.05
	ATOM	2426	С	SER A	338	59.769	34.255	26.613	1.00	21.75
	MOTA	2427	0	SER A	338	58.915	33.383	26.425	1.00	19.44
35	ATOM	2428	N	PHE A	339	60.093	35.154	25.681	1.00	24.18

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	- ATOM	2429	CA	PHE	A 339	59.444	35.141	24.371	1.00 24.18	
	ATOM	2430	СВ	PHE	A 339	59.962	36.276	23.467	1.00 24.91	
	MOTA	2431	CG	PHE	A 339	59.313	36.275	22.100	1.00 26.05	
	MOTA	2432	CD1	PHE	A 339	60.085	36.296	. 20.943	1.00 25.96	
5	ATOM	2433	CD2	PHE	A 339	57.934	36.251	21.977	1.00 25.69	•
	MOTA	2434	CE1	PHE	A 339	59.489	36.301	19.696	1.00 24.85	
	MOTA	2435	CE2	PHE	A 339	57.330	36.253	20.730	1.00 25.53	
	MOTA	2436	CZ	PHE	A 339	58.112	36.281	19.590	1.00 23.89	
	ATOM	2437	С	PHE	A 339	59.675	33.805	23.693	1.00 22.02	
10	MOTA	2438 .	0	PHE	A 339	58.812	33.305	22.995	1.00 22.73	•
	ATOM	2439	N	PHE	A 340	60.853	33.242	23.904	1.00 22.97	
	ATOM	2440	CA	PHE	A 340	61.213	31.964	23.299	1.00 23.44	
	MOTA	2441	СВ	PHE	A 340	62.696	31.959	22.954	1.00 21.17	
•	ATOM	2442	CG	PHE	A 340	63.108	33.128	22.105	1.00 18.96	
15	ATOM	2443	CD1	PHE	A 340	62.623	33.269	20.811	1.00 15.28	
	ATOM	2444	CD2	PHE	A 340	63.983	34.082	22.598	1.00 16.96	
	ATOM	2445	CE1	PHE	A 340	63.013	34.338	20.034	1.00 16.19	
	ATOM	2446	CE2	PHE	A 340	64.375	35.156	21.825	1.00 16.66	
	ATOM	2447	CZ	PHE	A 340	63.886	35.282	20.534	1.00 17.00	
20	ATOM	2448	С	PHE	A 340	60.855	30.741	24.156	1.00 26.22	
	ATOM	2449	0	PHE	A 340	61.224	29.616	23.806	1.00 26.38	
	ATOM	2450	N	ASP	A 341	60.136	. 30.952	25.272	1.00 28.20	
	MOTA	2451	CA	ASP	A 341	59.744	29.840	26.150	1.00 27.65	
	ATOM ·					58.830	30.323	27.290	1.00 28.09	
25	ATOM	2453	CG	ASP	A 341	59.562	31.111	28.373	1.00 28.12	
	MOTA	2454	OD1	ASP	A 341	60.796	30.975	28.498	1.00 27.75	
	ATOM	2455	OD2	ASP	A 341	58.892	31.868	29.098	1.00 30.69	
	MOTA	2456	С	ASP	A 341	59.033	28.755	25.367	1.00 28.02	
•	MOTA	2457	0	ASP	A 341	59.270	27.565	25.583	1.00 29.18	
30	ATOM	2458	N	GLU	A 342	58.156	29.163	24.451	1.00 28.63	
	MOTA	2459	CA	GLU	A 342	57.415	28.198	23.640	1.00 27.71	
	MOTA	2460	CB.	GLU	A 342	56.547	28.896	22.599	1.00 28.66	
	ATOM	2461	CG	GLU	A 342	55.801	27.939	21.678	1.00 29.56	
•	ATOM	2462	CD	GLU	A 342	54.648	28.595	20.949	1.00 30.24	
35	MOTA	2463	OE1	L GLU	A 342	53.632	27.909	20.714	1.00 33.64	

	ATOM	2464	OE2	GLU	A	342	54.756	29.794	20.612	1.00	31.91
	MOTA	2465	С	GLU	A	342	58.352	27.192	22.984	1.00	27.16
	ATOM	2466	0	GLU	A	342	58.122	25.997	23.054	1.00	28.46
	MOTA	2467	N	LEU	A	343	59.422	27.681	22.363	1.00	27.00
5	ATOM	2468	CA	LEU	A	343	60.393	26.802	21.718	1.00	26.58
,	'MOTA	2469	СВ	LEU	A.	343	61.505	27.629	21.060	1.00	25.90
	ATOM	2470	CG	LEU	A	343	61.058	28.712	20.058	1.00	26.74
	ATOM	2471	CD1	LEU	A	343	62.260	29.339	19.374	1.00	23.52
•	MOTA	2472	CD2	LEU	A	343	60.089	28.140	19.028	1.00	22.74
10	ATOM	2473	С	LEU	A	343	60.999	25.806	22.715	1.00	28.14
	MOTA	2474	O.	LEU	A	343	61.486	24.744	22.326	1.00	28.82
	ATOM	2475	N .	ARG	A	344	60.981	26.173	23.998	1.00	29.57
	·ATOM ·	2476	.CA	ARG	A	344	61.538	25.353	25.070	1.00	30.15
	MOTA	2477	CB	ARG	A	344	61.884	26.262	26.256	1.00	29.53
15	ATOM	2478	CG	ARG	A	344	63.311	26.106	26.754	1.00	25.45
	MOTA	2479	CD	ARG	A	344	64.113	27.395	26.664	1.00	21.49
	MOTA	2480	NE	ARG	A	344	63.314	28.608	26.901	1.00	18.01
	ATOM'	2481	CZ	ARG	A	344	63.742	29.830	26.603	1.00	13.11
	ATOM	2482	NHl	ARG	A	344	64.917	29.999	26.036	1.00	15.16
20	ATOM	2483	NH2	ARG	A	344	63.002	30.887	26.875	1.00	16.28
	ATOM	2484	С	ARG	A	344	60.571	24.249	25.515	1.00	31.98
	ATOM	2485	0	ARG	A	344	60.982	23.281	26.150	1.00	33.79
	ATOM	2486	N	ASP	A	345	59.293	24.406	25.180	1.00	33.25
	ATOM	2487	ĊĀ	ASP	À	345	58.242	23.449	25.530	1.00	35.71
25	ATOM	2488	CB	ASP	A	345	56.883	24.041	25.124	1.00	36.83
	ATOM	2489	CG	ASP	A	345	55.660	23.265	25.591	1.00	37.61
	MOTA	2490	OD1	ASP	A	345	54.573	23.873	25.653	1.00	39.11
	ATOM	2491	OD2	ASP	A	345	55.774	22.056	25.871	1.00	39.24
	ATOM	2492	С	ASP	A	345	58.463	22.077	24.863	1.00	37.75
30	MOTA	2493	0	ASP	A	345	58.633	21.987	23.647	1.00	37.67
	MOTA	2494	N	PRO	A	346	58.451	20.981	25.662	1.00	38.99
	MOTA	2495	CD	PRO	A	346	58.238	20.989	27.122	1.00	38.44
	MOTA	2496	CA	PRO	A	346	58.638	19.614	25.145	1.00	39.68
	MOTA	2497	CB	PRO	A	346	58.533	18.726	26.396	1.00	39.31
35	MOTA	2498	CG	PRO	A	346	58.747	19.646	27.551	1.00	38.56

	ATOM	2499	С	PRO A 346	57.539	19.243	24.155	1.00 40.56	
	ATOM.	2500	0	PRO A 346	57.758	18.461	23.228	1.00 40.27	•
	MOTA	2501	N	ASN A 347	56.358	19.760	24.424	1.00 42.43	3
	ATOM	2502	CA	ASN A 347	55.205	19.522	23.560	1.00 44.15	
5	MOTA	2503	CB	ASN A 347	53.928	19.386	24.364	1.00 45.69)
	ATOM	2504	CG	ASN A 347	54.183	3 18.874	25.759	1.00 46.82	2
	MOTA	2505	OD1	ASN A 347	54.107	19.621	26.717	1.00 48.40)
	MOTA	2506	ND2	ASN A 347	54,478	3 17.585	25.876	1.00 46.44	
	ATOM	2507	С	ASN A 347	55.101	20.648	22.557	1.00 45.30)
10	ATOM	2508	0	ASN A 347	54.367	21.603	22.772	1.00 45.75	5
	MOTA	2509	N	VAL A 348	55.800	20.568	21.428	1.00 46.70)
	ATOM	2510	CA	VAL A 348	55.825	21.669	20.449	1.00 46.47	1
	ATOM	2511	CB	VAL A 348	57.250	22.264	20.391	1.00 46.04	1
	ATOM	2512	CG1	VAL A 348	57.185	5 23.712	19.955	1.00 44.04	1
. 15	ATOM	2513	CG2	VAL A 348	57.97	22.124	21.725	1.00 44.33	:
·	ATOM	2514	С	VAL A 348	55.53	7 21.252	19.033	1.00 47.50	5
	MOTA	2515	0	VAL A 348	54.408	3 21.144	18.578	1.00 49.6	7
•	ATOM	2516	N	LYS A 349	56.733	3 21.027	18.372	1.00 49.0	7
	ATOM	2517	CA	LYS A 349	56.978	3 20.595	16.967	1.00 49.7	4
20	ATOM	2518	CB	LYS A 349	56.74	1 19.087	16.859	1.00 51.6	7
	MOTA	2519	CG	LYS A 349	55.34	4 18.739	17.305	1.00 53.90)
	MOTA	2520	CD	LYS A 349	54.80	9 17.547	16.564	1.00 56.03	3
	MOTA	2521	CE	LYS A 349	54.85	3 16.307	17.446	1.00 58.2	7 .
	ATOM	2522	NZ	LYS A 349	54.17	4 15.146	16.799	1.00 61.2	8
25	ATOM	2523	С	LYS A 349	56.02	2 21.275	16.040	1.00 48.9	5
•	MOTA	2524	0	LYS A 349	54.97	9 20.700	15.716	1.00 48.9	9
	ATOM	2525	N	LEU A 350	56.32	7: 22.484	15.565	1.00 47.7	4
	ATOM	2526	CA	LEU A 350	55.06	6 23.026	15.181	1.00 46.5	1
	ATOM	2527	СВ	LEU A 350	54.85	6 24.259	16.052	1.00 46.8	3
30	MOTA	2528	CG	LEU A 350	53.56	0 24.260	16.887	1.00 46.9	4
	ATOM	2529	CD1	LEU A 35	53.84	1 24.613	18.334	1.00 47.8	0
	MOTA	2530	CD2	LEU À 35	0 52.55	5 25.234	16.283	1.00 47.6	6
	MOTA	2531	С	LEU A 35	0 54.46	0 23.377	13.853	1.00 45.9	2
	MOTA	2532	0	LEU A 35	0 53.64	7 22.581	.13.380	1.00 46.1	0
35	MOTA	2533	N	PRO A 35	1 54.75	9 24.499	13.169	1.00 45.1	1
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•	MOTA	2534	CD	PRO A	351	55.423	25.732	13.632	1.00	44.07
	ATOM	2535	CA	PRO A	351	53.722	24.809	12.154	1.00	44.28
	MOTA	·2536	CB	PRO A	351	54.397	25.950	11.411	1.00	42.95
	ATOM	2537	CG	PRO A	351	55.110	26.705	12.512	1.00	43.47
5 ·	ATOM	2538	С	PRO A	351	53.060	23.662	11.434	1.00	43.92
	MOTA	2539	0	PRO A	35.1	51.833	23.548	11.439	1.00	45.39
	ATOM	2540	N	ASN A	352	53.870	22.805	10.828	1.00	44.49
	ATOM	2541	CA	ASN A	352	53.312	21.722	10.058	1.00	45.59
	ATOM	2542	CB	ASN A	352	53.931	21.727	8.659	1.00	45.84
10	MOTA	2543	CG	ASN A	352	53.124	22.481	7.640	1.00	48.02
	MOTA	2544	OD1	ASN A	352	53.320	22.301	6.443	1.00	49.81
	ATOM	2545	ND2	ASN A	352	52.225	23.327	8.109	1.00	47.62
	ATOM	2546	С	ASN A	352	53.596	20.357	10.683	1.00	46.48
	ATOM	2547	0	ASN A	352	53.398	20.154	11.889	1.00	46.98
15	ATOM	2548	N	GLY A	353	54.074	19.429	9.862	1.00	45.86
•	ATOM	2549	CA	GLY A	353	54.395	18.106	10.351	1.00	47.10
	ATOM	2550	С	GLY A	353	55.887	17.913	10.413	1.00	47.56
	MOTA	2551	0	GLY A	353	56.418	16.955	9.851	1.00	48.69
	ATOM	2552	· N	ARG A	354	56.567	18.848	11.074	1.00	47.79
20	ATOM	2553	CA	ARG A	354	58.015	18.803	11.181	1.00	48.26
	ATOM	2554	CB	ARG A	354	58.631	19.909	10.318	1.00	50.37
	MOTA	2555	CG	ARG A	354	58.796	19.527	8.849	1.00	53.05
	MOTA	2556	CD	ARG A	354 .	57.593	19.956	8.003	1.00	55.20
	MOTA	2557	NE	ARG A	354	57.294	21.393	8.135	1.00	56.34
25	ATOM	2558	CZ	ARG A	354	57.192	22.256	7.105	1.00	57.36
	MOTA	2559	NHl	ARG A	354	57.322	21.841	5.845	1.00	57.10
	ATOM .	2560	NH2	ARG A	354	56.944	23.547	7.341	1.00	57.28
	MOTA	2561	C	ARG A	354	58.480	18.961	12.622	1.00	47.05
	ATOM	2562	0	ARG A	. 354	57.901	19.724	13.396	1.00	46.38
30	MOTA	2563	N	ASP A	. 355	59.547	18.244	12.964	1.00	45.55
	ATOM	2564	CA	ASP A	355	60.110	18.318	14.298	1.00	43.83
	MOTA	2565	CB	ASP A	355	61.035	17.126	14.621	1.00	44.55
	MOTA	2566	CG	ASP A	355	61.108	16.051	13.547	1.00	44.92
	MOTA	2567	OD1	ASP A	355	60.108	15.328	13.356	1.00	43.70
35	MOTA	2568	OD2	ASP A	355	62.178	15.920	12.909	1.00	46.40

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		MOTA	2569	C .	ASP A	355	60.	.879	19.619	14.459	1.00	43.16			
		MOTA	2570	0	ASP A	355	61	.408	20.168	13.487	1.00	43.03			
		ATOM	2571·	N	THR A	356	60.	. 945	20.101	15.689	1.00	40.81	•	•	
		ATOM	2572	CA	THR A	356	61	.661	21.326	15.987	1.00	38.24			
	5	ATOM	2573	CB	THR A	356 _.	61.	.513	21.676	17.480	1.00	38.43			
		ATOM .	2574	OG1	THR A	356	62	. 687	22.274	18.Ò02	1.00	37.98			
•		ATOM	2575	CG2	THR A	356	61.	.161	20.496	18.364	1.00	37.12			
		ATOM	2576	С	THR A	356.	63.	.135	21.167	15.607	1.00	37.28			
	•	ATOM	2577	0	THR A	356	63	.755	20.154	15.932	1.00	36.68			
	10	ATOM	2578	N	PRO A	357	. 63	.715	22.160	14.901	1.00	35.88 ⁻			
		ATOM	2579	CD	PRO A	357	-63	.051	23389	14.448	1.00	34.92			
•	,	ATOM	2580	CA	PRO A	357	65.	.119	22.109	14.488	1.00	35.32·			
		MOTA	2581	CB	PRO A	357	65	. 376	23.464	13.818	1.00	35.57			
		ATOM	2582	CG	PRO A	357	64	.201	24.316	14.172	1.00	35.66			
	15	MOTA	2583	С	PRO A	357	66	.043	21.909	15.684	1.00	36.40			
		ATOM	2584	0	PRO A	357	65	. 604	21.957	16.836	1.00	36.57			
		MOTA	2585	N	ALA A	358	67	.311	21.653	15.401	1.00	36.04			
		ATOM	2586	CA	ALA A	358	68	.308	21.399	16.430	1.00	36.22			
		ATOM	2587	CB	ALA A	358	69	.566	20.801	15.822	1.00	37.16			
	20	ATOM	2588	С	ALA A	358	. 68	.647	22.610	17.308	1.00	36.38			
		MOTA	2589 [°]	0	ALA A	358	69	.722	23.196	17.186	1.00	37.29			
		MOTA	2590	N	LEU A	359	67	.758	22.931	18.240	1.00	35.60	•		
		MOTA	2591	CA	LEU A	·359	68	.011	24.004	19.186	1.00	35.86			
		MOTA	2592	CB	LEU A	359	66	.750	24.827	19.489	1.00	34.90			
	25	ATOM .	2593	CG	LEU A	359	65	.744	25.034	18.349	1.00	35.74		•	
		ATOM	2594	CD1	LEU A	359	64	.380	25.401	18.924	1.00	36.49			
		ATOM	2595	CD2	LEU A	359	66	.220	26.108	17.378	1.00	33.17			
•		ATOM	2596	C	LEU A	359	68	.539	23.355	20.470	1.00	36.74			
		MOTA	2597	0	LEU A	359	68	.464	22.121	20.625	1.00	38.67			
	30	ATOM	2598	N	PHE A	360	69	.073	24.154	21.384	1.00	35.31			
		MOTA	2599	CA	PHE A	360	69	.604	23.599	22.639	1.00	33.68			
		ATOM	2600	CB	PHE A	360	68	.592	22.645	23.297	1.00	29.33			
•		ATOM	2601	CG	PHE A	360	67	.151	23.028	23.092	i.00	25.75			
		MOTA	2602	CD1	PHE A	360	66	.215	22.074	22.745	1.00	24.32			
	35	MOTA	2603	CD2	PHE A	360	. 66	.737	24.340	23.245	1.00	23.11			
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		•													
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	ATOM	2604	CE1	PHE	A	360	64.893	22.416	22.557	1.00	22.23
	ATOM	2605	CE2	PHE	A	360	65.415	24.688	23.058	1.00	21.69
	ATOM	2606	CZ	PHE	A	360	64.493	23.723	22.714	1.00	22.31
	ATOM	2607	C	PHE	A	360	70.938	22.890 .	22.401	1.00	34.08
5	ATOM	2608	0	PHE	A	360	71.581	22.413	23.338	1.00	34.63
	ATOM	2609	N	ASN	A	361	71.348	22.863	21.132	1.00	35.29
	ATOM	2610	CA	ASN	A	361	72.609	22.265	20.670	1.00	35.58
	ATOM	2611	CB	ASN	A	361	72.640	22.420	19.139	1.00	36.74
	ATOM	2612	CG	ASN	A	361	73.165	21.225	18.392	1.00	38.91
10	ATOM .	2613	OD1	ASN	A	361	73.503	20.205	18.986	1.00	42.48
	MOTA	2614	ND2	ASN	A	361	73.235	21.347	17.069	1.00	39.99
	ATOM	2615	С	ASN	A	361	73.830	23.005	21.272	1.00	34.58
	ATOM	2616	0	ASN	Ά	361 ⁻	74.969	22.786	20.853	1.00	33.31
	ATOM	2617	N	PHE	A	362	73.567	23.870	22.265	1.00	33.34
15	ATOM	2618	CA	PHE	A	362	74.595	24.720	22.895	1.00	30.24
	ATOM	2619	CB	PHE	A	362	74.044	25.448	24.128	1.00	26.30
	ATOM	2620	CG	PHE	A	362	73.059	26.527	23.796	1.00	24.99
	ATOM	2621	CD1	PHE	A	362	71.710	26.344	24.031	1.00	24.49
	ATOM	2622	CD2	PHE	A	362	73.480	27.724	23.233	1.00	24.20
20	MOTA	2623	CE1	PHE	A	362	70.797	27.336	23.704	1.00	25.12
	MOTA	2624	CE2	PHE	À	362	72.571	28.716	22.909	1.00	22.66
	MOTA	2625	CZ	PHE	A	362	71.231	28.521	23.141	1.00	21.69
	MOTA	2626	С	PHE	A	362	75.863	23.960	23.252	1.00	29.70
	ATOM	2627	0	PHE	A	362	75.833	22.787	23.624.	.1.00	31.38
25	MOTA	2628	N	THR	A	363	76.973	24.666	23.115	1.00	28.72
	ATOM	2629	CA	THR	A	363	78.283	24.139	23.426	1.00	30.32
	ATOM	2630	CB	THR	A	363	79.118	23.949	22.160	1.00	30.33
-	ATOM	2631	OG1	THR	A	363	79.626	25.227	21.730	1.00	29.69
	ATOM	2632	CG2	THR	A	363	78.264	23.324	21.073	1.00	31.54
30	ATOM	2633	С	THR	A	363	78.993	25.132	24.285	1.00	29.90
	MOTA	2634	0	THR	A	363	78.570	26.284	24.450	1.00	31.27
•	MOTA	2635	N	THR	A	364	80.157	24.708	24.797	1.00	31.32
	MOTA	2636	CA	THR	A	364	80.885	25.620	25.708	1.00	31.31
	ATOM	2637	CB	THR	A	364	82.183	25.077	26.188	1.00	31.99
35	MOTA	2638	OG1	THR	A	364	81.967	23.911	26.995	1.00	33.21

	MOTA	2639	CG2	THR A	364	82.909	26.131	26.996	1.00	32.54
	ATOM	2640	C	THR A	364	81.244	26.991	25.221	1.00	31.22
	MOTA	2641	0	THR A	364	80.931	27.967	25.917	1.00	32.20
	ATOM	2642	N	GLN A	. 365	81.864	27.183	24.096	1.00	31.18
5	ATOM	2643	CA	GLN A	365	82.097	28.555	23.672	1.00	29.69
	MOTA	2644	CB	GLN A	. 365 ·	82.591	28.657	22.225	1.00	31.29
	ATOM	2645	CG	GLN A	365	84.066	28.448	22.048	1.00	31.31
	ATOM	2646	CD	GLN A	365	84.834	29.709	21.698	1.00	28.08
	ATOM	2647	OE1	GLN A	365	84.239	30.773	21.479	1.00	27.43
10	ATOM	2648	NE2	GLN A	365	86.156	29.819	21.590	1.00	32.84
	ATOM	2649	C	GLN A	365	80.809	29.336	23.556	1.00	27.35
	ATOM	2650	0	GLN A	365	80.758	30.523	23.902	1.00	27.88
	MOTA	2651	N	GLU A	366	79.767	28.699	23.081	1.00	25.28
	MOTA	2652	CA	GLU A	366	78.560	29.472	22.934	1.00	26.02
15	ATOM	2653	CB	GLU A	366	77.497	28.614	22.291	1.00	24.56
	MOTA	2654	CG	GLU A	366	77.570	28.538	20.791	1.00	23.39
	MOTA	· 2655	CD	GLU P	366	76.295	27.905	20.307	1.00	20.84
	MOTA	2656	OE1	GLU A	366	75.379	28.656	19.899	1.00	18.16
	ATOM	2657	OE2	GLU F	366	76.200	26.667	20.333	1.00	21.04
20	MOTA	2658	С	GLU F	A 366	78.018	30.001	24.257	1.00	25.56
	ATOM	2659	0	GLU F	A 366	77.440	31.086	24.316	1.00	26.33
	MOTA	2660	N	LEU A	A 367 .	78.235	29.243	25.311	1.00	27.66
	MOTA	2661	CA	LEU A	A 367	77.747	29.637	26.617	1.00	27.22
	ATOM	2662	CB	LEU A	A 367	77.389	28.409	27.463	1.00	23.10
25	MOTA	2663	CG	LEU A	A 367	76.197	27.579	26.998	1.00	22.63
	MOTA	2664	CD1	LEU A	A 367	76.279	26.163	27.553	1.00	24.80
	MOTA	2665	CD2	LEU I	A 367	74.886	28.228	27.395	1.00	22.27
	ATOM	2666	С	LEU A	A 367	78.782	30.491	27.342	1.00	27.79
	ATOM	2667	0	LEU I	A 367	78.474	31.114	28.368	1.00	29.77
30	MOTA	2668	N	SER	A 368	80.017	30.518	26.796	1.00	28.63
	MOTA	2669	CA	SER .	A 368	81.163	31.252	27.355	1.00	30.09
	MOTA	2670	CB	SER .	A 368	82.311	31.408	26.353	1.00	30.06
	MOTA	2671	OG	SER	A 368	82.146	32.543	25.524	1.00	32.28
	MOTA	2672	C	SER	A 368	80.794	32.563	28.040	1.00	31.79
35	MOTA	2673	0	SER	A 368	81.462	32.988	28.998	1.00	32.23

	ATOM	2674	N	SER A	Ą	369	79.711	33.174	27.586	1.00	31.30
	ATOM .	2675	CA	SER A	Ą	369	79.225	34.393	28.200	1.00	31.27
	MOTA	2676	CB	SER I	A	369	78.832	35.437	27.141	1.00	28.64
	ATOM	2677	OG	SER Z	A	369	77.432	35.662	27.104	1.00	23.51
5	ATOM	2678	С	SER A	A	369	78.040	34.011	29.084	1.00	33.13
	ATOM	2679	0	SER 2	A	369	76.968	33.649	28.587	1.00	37.45
	ATOM	2680	N	ASN 2	A	370	78.237	34.040	30.384	1.00	31.36
	ATOM	2681	CA	ASN 3	A	370	77.172	33.659	31.306	1.00	29.84
	ATOM ·	2682	CB	ASN A	A	370	75.917	34.511	31.061	1.00	31.79
10	ATOM	2683	CG	ASN I	A	370	75.177	34.854	32.344	1.00	32.69
	ATOM	2684	OD1	ASN I	A	370	74.323	35.750	32.368	1.00	33.79
	ATOM	2685	ND2	ASN	A	370	75.498	34.140	33.414	1.00	30.98
	ATOM	2686	С	ASN .	A	370	76.835	32.155	31.241	1.00	26.34
	ATOM	2687	0	ASN .	A	370	75.697	31.774	30.963	1.00	27.40
15	ATOM	2688	N	PRO .	A	371	77.815	31.278	31.516	1.00	24.52
	ATOM	2689	CD	PRO .	A	371	79.202	31.636	31.868	1.00	24.13
	MOTA	2690	.CA	PRO .	A	371	77.611	29.816	31.509	1.00	25.51
	ATOM	2691	CB	PRO	A	371	78.909	29.272	32.100	1.00	25.50
	ATOM	2692	CG	PRO	A	371	79.923	30.323	31.797	1.00	24.03
20	MOTA	2693	C.	PRO	À	371	76.371	29.337	32.309	1.00	26.66
	MOTA	2694	0	PRO	A	371	75.691	28.393	31.886	1.00	27.02
	MOTA	2695	N	PRO	A	372	76.052	29.960	33.478	1.00	27.86
	MOTA	2696	CD	PRO	A	372	76.803	31.069	34.108	1.00	28.58
	ATOM	2697	CA	PRO	A	372	74.879	29.570	34.295	1.00	28.30
25	ATOM	2698	CB	PRO	A	372	74.857	30.622	35.415	1.00	28.19
	ATOM	2699	CG	PRO	A	372	76.266	31.086	35.518	1.00	29.14
	ATOM	2700	C	PRO	A	372	73.564	29.642	33,508	1.00	28.82
	MOTA	2701	0	PRO	A	372	72.582	28.953	33.834	1.00	27.79
	ATOM	2702	N	LEU	A	373	73.544	30.479	32.466	1.00	28.69
30	ATOM	2703	CA	LEU	A	373	72.353	30.643	31.627	1.00	29.17
	ATOM	2704	CB	LEU	A	373	72.618	31.651	30.508	1.00	29.53
	MOTA	2705	CG	LEU	A	373	72.437	33.126	30.866	1.00	30.15
	ATOM	2706	CD1	LEU	A	373	72.479	33.987	29.604	1.00	31.19
	ATOM	2707	CD2	LEU	A	373	71.139	33.342	31.623	1.00	26.78
35	ATOM	2708	С	LEU	A	373	71.871	29.314	31.035	1.00	27.62

	MOTA	2709	0	LEU A	373	70.722	29.202	30.623	1.00	28.74
	ATOM	2710.	N	ALA A	374	72.754	28.314	31.005	1.00	28.72
	MOTA	2711	CA	ALA A	374	72.438	26.981	30.471	1.00	30.45
	ATOM	2712	CB .	ALA A	374	73.660	26.075	30.561	1.00	30.45
5	ATOM	2713	С	ALA A	374	71.227	26.313	31.142	1.00	31.42
	ATOM	2714	0	ALA A	374	70.521	25.522	30.507	1.00	31.67
	MOTA	2715	N	THR A	375	70.988	26.613	32.424	1.00	32.66
	ATOM	2716	CA	THR A	375	69.860	26.010	33.149	1.00	32.06
	ATOM	2717	СВ	THR A	375	69.942	26.279	34.659	1.00	33.87
10	ATOM	2718	OGl	THR A	375	69.884	27.667	34.951	1.00	36.94
	ATOM	2719	CG2	THR A	375	71.191	25.720	35.301	1.00	33.69
	MOTA	2720	C	THR A	375	68.518	26.438	32.567	1.00	31.74
	ATOM	2721	0	THR A	375	67.512	25.734	32.692	1.00	31.00
	ATOM	2722	N	ILE A	376	68.513	27.581	31.898	1.00	32.30
15	ATOM	2723	CA.	ILE A	376	67.300	28.075	31.261	1.00	32.02
	MOTA	2724	CB	ILE A	376	67.176	29.614	31.381	1.00	33.14
	ATOM	2725	CG2	ILE A	376	66.145	30.159	30.401	1.00	33.69
	MOTA	2726	CG1	ILE A	376	66.805	30.016	32.806	1.00	31.53
	ATOM	2727	CD1	ILE A	376	67.100	31.466	33.115	1.00	31.64
20	MOTA	2728	С	ILE A	376 ⁻	67.285	27.682	29.776	1.00	30.98
	MOTA	2729	0	ILE A	376	66.274	27.222	29.257	1.00	31.62
	MOTA	2730	N	LEU A	377	68.416	27.903	29.108	1.00	31.31
	MOTA	2731	CA	LEU A	377 .	68.582	27.635	27.672	1.00	31.31
	MOTA	2732	CB	LEU A	377	69.931	28.161	27.191	1.00	27.99
25	MOTA	2733	CG	LEU A	377	70.072	29.675	27.259	1.00	25.47
	ATOM	2734	CD1	LEU A	377	71.528	30.100	27.237	1.00	23.87
	ATOM	2735	CD2	LEU A	377	69.280	30.325	26.145	1.00	24.82
	ATOM	2736	С	LEU A	377	68.397	26.176	27.274	1.00	32.58
	MOTA	2737	0	LEU A	377	67.801	25.887	26.231	1.00	32.49
30	ATOM	2738	N	ILE A	378	68.920	25.264	28.092	1.00	33.25
	MOTA	2739	CA	ILE A	378	68.822	23.840	27.811	1.00	32.83
	MOTA	2740	CB	ILE A	378	70.186	23.137	27.968	1.00	30.55
	MOTA	2741	CG2	ILE A	378	70.072	21.663	27.607	1.00	30.53
	MOTA	2742	CG1	ILE A	. 378	71.238	23.830	27.090	1.00	29.45
35	MOTA	2743	CD1	ILE A	. 378	72.659	23.356	27.321	1.00	28.60

	ATOM	2744	C	ILE A	378	67.771	23.171	28.697	1.00	35.98
	ATOM	2745	0	ILE A	378	68.046	22.821	29.849	1.00	36.93
	ATOM	2746	N	PRO A	379	66.544	22.982	28.162	1.00	36.15
	MOTA	2747	CD	PRO A	379	66.146	23.369	26.796	1.00	36.55
5	ATOM	2748	CA	PRO A	.379	65.447	22.345	28.899	1.00	36.01
	MOTA	2749	CB T	PRO A	379	64.261	22.395	27.925	1.00	35.91
	MOTA	2750	CG	PRO A	379	64.863	22.617	26.579	1.00	36.09
-	MOTA	2751	С	PRO A	379	65.782 .	20.902	29.272	1.00	36.21
	ATOM	2752	0	PRO A	379	66.574	20.251	28.587	1.00	37.18
10	MOTA	2753	N	PRO A	. 380	65.192	20.394	30.387	1.00	36.38
	MOTA	2754	CD	PRO A	380	64.257	21.124	31.257	1.00	35.79
	ATOM	2755	CA	PRO A	380	65.431	19.029	30.895	1.00	35.56
	ATOM	2756	CB	PRO A	. 380	64.366	18.844	31.990	1.00	35.32
	ATOM	2757	CG	PRO A	. 380	63.444	20.013	31.859	1.00	35.77
15	ATOM	2758	C	PRO A	. 380	65.319	17.928	29.836	1.00	35.35
	ATOM	2759	0	PRO A	380	66.174	17.045	29.770	1.00	35.04
	· ATOM	2760	N	HIS A	381	64.269	17.975	29.019	1.00	36.71
	ATOM	2761	CA	HIS A	381	64.055	16.967	27.977	1.00	38.77
	ATOM	2762	СВ	HIS A	381	62.675	17.142	27.341	1.00	39.92
20	ATOM	2763	CG	HIS A	381	62.575	18.337	26.441	1.00	40.52
	ATOM	2764	CD2	HIS A	381	62.183	19.613	26.696	1.00	40.13
	ATOM	2765	NDl	HIS A	381	62.924	18.305	25.105	1.00	40.43
	ATOM	2766	CE1	HIS A	381	62.754	19.508	24.578	1.00	39.78
	ATOM	2767	NE2	HIS F	381	62.305	20.319	25.523	1.00	39.78
25	ATOM	2768	С	HIS F	381	65.135	16.982	26.886	1.00	40.47
•	ATOM	2769	0	HIS A	A 381	65.301	15.998	26.165	1.00	41.54
	ATOM	2770	N	ALA A	A 382	65.845	18.102	26.752	1.00	41.62
	ATOM	2771	CA	ALA A	A 382	66.883	18.250	25.729	1.00	43.15
	MOTA	2772	CB	.ALA A	A 382	66.857	19.662	25.151	1.00	42.23
30	ATOM	2773	- C.	ALA A	A 382	68.281	17.921	26.250	1.00	44.64
	ATOM	2774	0	ALA A	A 382	69.198	17.672	25.460	1.00	44.18
	ATOM	2775	N	ARG A	A 383	68.454	17.934	27.572	1.00	46.22
	ATOM	2776	CA	ARG A	A 383	69.757	17.648	28.167	1.00	47.97
	ATOM	2777	CB	ARG A	A 383	69.736	17.948	29.663	1.00	48.04
35	ATOM	2778	CG	ARG Z	A 383	69.744	19.445	29.958	1.00	49.84

	ATOM	2779	CD	ARG	A	383	69.740	19.742	31.451	1.00	49.31
	ATOM	2780	NE	ARG	A	383	68.841	20.849	31.789	1.00	50.09
	ATOM	2781	CZ	ARG	A	383	68.325	21.059	33,011	1.00	51.14
	MOTA	2782	NH1	ARG	A	383	68.671	20.282	.34.040	1.00	50.04
5	ATOM	2783	้ ทุ่หว	ARG	A	383	67.467	22.059	33.207	1.00	50.78
	ATOM	2784	С	ARG	A	383	70.202	16.208	27.888	1.00	49.14
	MOTA	2785	0	ARG	A	383	69.405	15.269	27.951	1.00	49.60
	MOTA	2786	N	ILE	A	384	71.485	16.064	27.544	1.00	50.06
	ATOM	2787	CA	ILE	A	384	72.086	14.770	27.210	1.00	51.09
10	ATOM	2788	CB	ILE	A	384	. 72.710	14.801	25.795	1.00	51.18
	ATOM	2789	CG2	ILE	A	384	72.959	13.393	25.280	1.00	52.93
	MOTA	2790	CG1	ILE	A	384	71.819	15.577	24.825	1.00	50.79
	ATOM	2791	CD1	ILE	A	384	72.542	16.695	24.105	1.00	52.35
	MOTA	2792	С	ILE	A	384	73.170	14.372	28.219	1.00	51.65
15	MOTA	2793	OT1	ILE	A	384	73.644	15.255	28.970	1.00	51.89
	ATOM	2794	OXT	ILE	A	384	73.537	13.175	28.250	1.00	52.45
	TER	2795		ILE	A	384					
	MOTA	2796	СВ	VAL	В	37	36.802	77.140	-23.975 ⁻	1.00	51.55
	MOTA	2797	CG1	VAL	В	37	35.939	76.007	-23.436	1.00	50.87
20	MOTA	2798	CG2	VAL	В	37	35.933	78.188	-24.660	1.00	51.89
	ATOM	2799	C .	VAL	В	37	38.541	76.737	-22.201	1.00	51.79
•	ATOM	2800	0	VAL	В	37	39.596	76.390	-22.744	1.00	52.10
•	ATOM	2801	N.	VAL	В	37 .	38.437	78.942	-23.333	1.00	51.63
•	ATOM	2802	CA	VAL	В	37	37.637	77.786	-22.844	1.00	51.54
25	ATOM	2803	N	THR	В	38	38.120	76.245	-21.032	1.00	51.45
	MOTA	2804	CA	THR	В	38	38.872	75.239	-20.274	1.00	49.87
	MOTA	2805	CB	THR	В	38	38.764	73.832	-20.899	1.00	50.03
	ATOM	2806	OG1	THR	В	38	39.783	72.969	-20.422	1.00	50.26
	MOTA	2807	CG2	THR	В	38	38.796	73.804	-22.412	1.00	50.44
30	MOTA	2808	С	THR	В	38	40.329	75.658	-20.045	1.00	48.71
	ATOM	2809	0	THR	В	38	41.244	75.175	20.712	1.00	49.59
	ATOM	2810	N	THR	В	39	40.526	76.558	-19.083	1.00	46.30
	ATOM	2811	CA	THR	В	39	41.852	77.053	-18.729	1.00	43.19
	MOTA	2812	CB	THR	В	.39	41.750	78.464	-18.147	1.00	43.29
35	ATOM	2813	OG1	THR	В	39	40.832	79.264	-18.874	1.00	44.92

	MOTA	2814	CG2	THR	В	39	43.072	79.196	-18.077	1.00	43.86
	MOTA	2815	С	THR	В	39 .	42.495	76.141	-17.695	1.00	41.22
	MOTA	2816	0	THR	В	39	41.838	75.709	-16.753	1.00	42.40
	ATOM	2817	N	VAL	В	40	43.783	75.871	-17.864	1.00	38.57
5	ATOM	2818	CA	VAL	В	40	44.520	75.032	-16.930	1.00	35.10
	ATOM	2819	CB	VAL	В	40	45.089	73.765	-17.593	1.00	34.50
	ATOM	2820	CG1	VAL	В	40	45.866	72.929	-16.583	1.00	34.63
	ATOM	2821 .	CG2	VAL	В	40	43.965	72.949	-18.199	1.00	32.73
	ATOM	2822	С	VAL	В	40	45.632	75.836	-16.278	.1.00	34.58
10	MOTA	2823	0	VAL	В	40	46.470	76.440	-16.961	1.00	34.85
	MOTA	2824	N	VAL	В	41	45.616	75.871	-14.953	1.00	31.60
	MOTA	2825	CA	VAL	В	41	46.603	76.629	-14.205	1.00	29.68
	MOTA	2826	CB	VAL	В	41	45.963	77.919	-13.625	1.00	30.25
	ATOM	2827	CG1	VAL	В	41	45.113	77.614	-12.395	1.00	30.02
15	ATOM	2828	CG2	VAL	В	41 ·	47.023	78.955	-13.300	1.00	31.38
	ATOM	2829	С	VAL	В	41	47.175	75.798	-13.066	1.00	27.96
	ATOM	2830	0	VAL	В	41	46.525	74.886	-12.576	1.00	26.60
	-ATOM	2831	N	ALA	В	42	48.373	76.145	-12.630	1.00	28.15
	MOTA	2832	CA	ALA	. В	42	48.993	75.450	-11.505	1.00	29.54
20	MOTA	2833	CB	ALA	В	42	50.484	75.244	-11.733	1.00	28.92
	ATOM	2834	С	ALA	В	42	48.742	76.280	-10.249	1.00	2948
	ATOM	2835	0	ALA	В	42	49.269	77.381	-10.122	1.00	28.42
	ATOM	2836	N	THE	В	43	47.904	75.767	-9.349	1.00	30.71
	ATOM .	2837	CA	THE	В	43	47.558	76.496	-8.120	1.00	33.11
25	MOTA	2838	CB	THE	B	43	46.168	77.126	-8.288	1.00	35.28
	MOTA	2839	OG1	THE	R B	43	45.614	77.507	-7.040		42.46
	MOTA	2840	CG2	2 THE	RB	43	45.166	76.232	-8.980	1.00	35.35
	ATOM	2841	С	THE	RB	43	47.569	75.605	-6.871	1.00	32.03
	MOTA	2842	0	TH	R B	43	47.210	74.437	-6.942	1.00	31.25
30	ATOM	2843	N	PR	D B	44	48.002	76.153	-5.704	1.00	32.19
	ATOM	2844	CD	· PR	O B	44	48.501	77.503	-5.521	1.00	34.09
	ATOM	2845	CA	PR	ОВ	44	48.067	75.431	-4.431	1.00	32.79
	MOTA	2846	СВ	PR	ОВ	44	49.192	76.165	-3.672	1.00	32.20
	ATOM	2847	CG	PR	ОВ	44	49.639	77.267	-4.578	1.00	31.97
35	ATOM	2848	С	PR	ОВ	44	46.773	75.558	3 -3.632	1.00	31.84

	MOTA	2849	0	PRO !	В	44	46.	099	76.586	-3.680	1.00	28.42
	ATOM	2850	И.	GLY :	В	45	46.	452	74.512	-2.872	1.00	35.47
	ATOM	2851	CA	GLY :	В	45	45.	257	74.538	-2.036	1.00	39.23
	ATOM	2852	Ç.	GLY :	В	45	45.	504	75.287	-0.729	1.00	41.21
5	ATOM	2853	0	GLY	В	45	46.	462	76.060	-0.623	1.00	38.55
	ATOM	2854	N	GLN	В	46	44.	650	75.046	0.274	1.00	46.75
	ATOM	2855	CA	GLN	В	46	44.	793	75.693	1.588	1.00	48.74
	ATOM	2856	СВ	GLN	В	46	43.	484	76.341	2.035	1.00	50.72
	ATOM	2857	CG	GLN	В	46	42.	261	75.448	1.895	1.00	53.41
10	ATOM	2858	CD	GLN	В	46	41.	.122	75.883	2.795	1.00	53.10
	ATOM	2859	OE1	GLN	В	46	40	.767	77.064	2.841	1.00	53.10
	ATOM	2860	NE2	GLN	В	46	40	.544	74.926	3.518	1.00	53.76
	ATOM	2861	Ç	GLN	В	46	45	.320	74.716	2.647	1.00	50,13
	MOTA	2862	Ο.	GLN	В	46	44	.619	74.359	3.603	1.00	50.65
15	MOTA	2863	N	GLY	В	47	46	.570	74.298	2.458	1.00	50.48
	MOTA	2864	CA	GLY	В	47	47	.236	73.375	3.366	1.00	51.37
	MOTA	2865	С	GLY	B	47	48	.740	73.407	3.156	1.00	51.41
	MOTA	2866	0	GLY.	В	47 -	49	.328	74.487	3.092	1.00	52.08
	ATOM	. 2867	N	PRO	В	48	49	.339	72.184	2.925	1.00	51.20
20	MOTA	2868	CD	PRO	В	48	49	.147	71.119	3.933	1.00	51.98
	ATOM	2869	CA	PRO	В	48	50	.809	71.950	2.537	1.00	50.93
	ATOM	2870	СВ	PRO	В	48	50	.961	70.469	2.445	1.00	51.77
••	ATOM	2871	CG	PRO	В	48	50	.174	70.062	3.621	1.00	51.47
	ATOM	2872	С	PRO	В	48	51	.163	72.527	1.240	1.00	49.84
25	MOTA	2873	0	PRO	В	48	51	.079	71.800	0.266	1.00	50.79
	MOTA	2874	N	ASP	В	49	51	.537	73.731	1.055	1.00	48.06
	MOTA	2875	CA	ASP	В	49	51	.732	74.195	-0.333	1.00	47.60
	MOTA	2876	CB	ASP	В	49	53	.022	74.936	-0.423	1.00	48.55
	MOTA	2877	CG	ASP	В	49	52	.835	.76.305	0.221	1.00	50.19
30	ATOM	2878	OD1	ASP	В	49	52	.171	77.158	-0.396	1.00	52.20
	ATOM	2879	OD2	2 ASP	В	49	53	.335	76.504	1.351	1.00	51.50
	MOTA	2880	С	ASP	В	49	51	.479	73.199	-1.498	1.00	45.81
	ATOM	2881	0	ASP	В	49	50	.386	73.28	7 -2.046	1.00	45.95
	ATOM	2882	N	ARG	В	, 50	52	.319	72.25	7 -1.958	1.00	42.31
35	MOTA	2883	CA	ARG	В	50	51	892	71.32	7 -3.084	1.00	40.48

•	ATOM	2884	CB	ARG	B	50	51.271	70.083	-2.442	1.00	41.47
	MOTA	2885	CG	ARG	В	50	50.732	69.037	-3.397	1.00	44.10
•	MOTA	2886	CD	ARG	В	50	50.762	67.634	-2.780	1.00	46.35
	MOTA	2887	NE	ARG	B	50	49.679	67.438	-1.813	1.00	51.22
5	ATOM	2888	CZ	ARG	В	50	49.855	67.035	-0.542	1.00	51.26
•	MOTA	2889	NH1	ARG	В	50	51.069	66.787	-0.075	1.00	51.16
	ATOM	2890	NH2	ARG	В	50	48.804	66.876	0.261	1.00	51.87
	ATOM	2891	С	ARG	в.	50	50.922	71.887	-4.203	1.00	35.73
	ATOM	2892	0	ARG	В	50	49.752	71.523	-4.252	1.00	34.77
10	MOTA	2893	N	PRO	В	51	51.446	72.766	-5.084	1.00	33.78
•	MOTA	2894	CD	PRO	В	51	52.801	73.315	-4.963	1.00	33.89
	ATOM	2895	CA	PRO	В	51	50.736	73.310	-6.258	1.00	33.19
	ATOM	2896	CB	PRO	В	51	51.750	74.263	-6.894	1.00	31.56
	MOTA	2897	CG	PRO	В	51	52.736	74.552	-5.816	1.00	33.65
15	ATOM	2898	.C	PRO	В	51	50.373	72.199	7.238 ·	1.00	31.20
٠	MOTA	2899	0	PRO	В	51	51.215	71.378	-7.590	1.00	33.41
•	MOTA	2900	N	GĻN	В	52	49.115	72.159	-7.645	1.00	30.94
	MOTA	2901	CA	GLN	В	52	48.631	71.128	-8.559	1.00	30.72
	ATOM	2902	СВ	GLN	В	52	47.668	70.192	-7.822	1.00	32.26
20	ATOM	2903	CG	GLN	В	52	46.545	70.921	-7.099	1.00	34.16
	ATOM	2904	CD	GLN	В	52	45.411	70.001	-6.697	1.00	37.58·
	ATOM	2905	OE1	GLN	В	52	44.489	69.751	-7.480	1.00	39.21
	ATOM	2906	NE2	GLN	В	52	45.466	69.492	-5.466	1.00	38.21
	ATOM	2907	С	GLN	В	52	47.933	71.726	-9.785	1.00	29.17
25	ATOM	2908	0 .	GLN	В	52	47.461	72.863	-9.763	1.00	26.63
	MOTA	2909	N	GLU	В	53	47.858	70.940	-10.851	1.00	29.44
	ATOM	2910	CA	GLU	В	53	47.206	71.378	-12.086	1.00	29.61
	ATOM	2911	CB	GLU	В	53	47.528	70.400	-13.220	1.00	30.96
	ATOM	2912	CG	GLU	В	53 .	48.757	70.782	-14.031	1.00	33.49
30	MOTA	2913	CD	GLU	В	53	48.861	70.022	-15.351	1.00	36.32
	MOTA	2914	OE1	GLU	В	53	49.955	69.489	-15.639	1.00	35.83
	MOTA	2915	OE2	GLU	В	53	47.849	69.963	-16.098	1.00	36.83
	MOTA	2916	С	GLU	В	53	45.693	71.502	-11.900	1.00	28.07
	MOTA	2917	0	GLU	В	53	45.045	70.562	-11.459	1.00	29.41
35	MOTA	2918	N	VAL	В	54	45.138	72.674	-12.234	1.00	27.34

	MOTA	2919	CA	VAL E	В	54	43.701	72.922	-12.096	1.00	27.42
	MOTA	2920	СВ	VAL E	В	54	43.395	73.879	-10.921	1.00	26.77
	MOTA	2921	CG1	VAL E	В	54	41.970	74.411	-11.018	1.00	26.06
	ATOM	2922	CG2	VAL I	В	54	43.608	73.179	9.586	1.00	28.23
5	ATOM	2923	С	VAL E	В	54	43.110	73.507	-13.382	1.00	28.07
	ATOM	2924	0	VAL I	В	54	43.619	74.490	-13.924	1.00	30.35
	ATOM	2925	N	SER I	В	55	42.033	72.900	-13.861	1.00	28.47
	ATOM	2926	CA	SER E	В	55	41.378	73.363	-15.083	1.00	29.26
	ATOM	2927	CB	SER F	В	55	41.358	72.252	-16.140	1.00	27.83
10	ATOM	2928	OG	SER I	В	55	42.566	71.509	-16.135	1.00	30.97
	MOTA	.2929	С	SER I	В	55	39.963	73.853	-14.815	1.00	28.63
	ATOM	2930	0	SER I	В	55	39.209	73.238	-14.063	1.00	29.48
	ATOM	2931	N	TYR I	В	56	39.600	74.958	-15.447	1.00	29.65
	ATOM	2932	CA	TYR I	В	56	38.267	75.513	-15.286	1.00	31.29
15	ATOM	2933	CB	TYR I	В	56	38.209	76.490	-14.110	1.00	29.12
	MOTA	2934	CG	TYR I	В	56	39.108	77.699	-14.233	1.00	26.96
	ATOM	2935	CD1	TYR I	В	56	40.371	77.712	-13.651	1.00	27.72
	ATOM	2936	CE1	TYR I	В	56	41.183	78.825	-13.737	1.00	27.52
	MOTA	2937	CD2	TYR !	В	56	38.686	7,8.833	-14.903	1.00	24.94
20	MOTA	2938	CE2	TYR I	В	56	39.495	79.947	-14.998	1.00	26.38
	MOTA	2939	CZ	TYR	В	56	40.740	79.940	-14.413	1.00	26.96
	MOTA	2940	ОН	TYR 1	В	56	41.544	81.057	-14.497	1.00	29.38
	ATOM	2941	C ·	TYR :	В	56	37.792	76.184	-16.561	1.00	32.84
	ATOM	2942	0	TYR	B	56	38.585	76.736	-17.311	1.00	34.73
25	ATOM	2943	N	THR	В	57.	36.495	76.137	-16.798	1.00	35.16
	ATOM	2944	CA	THR	В	57	35.925	76.747	-17.988	1.00	37.24
	ATOM	2945	CB	THR	В	57	35.620	75.668	-19.030	1.00	36.42
•	ATOM	2946	OG1	THR	В	57 ·	35.393	76.247	-20.300	1.00	38.30
	MOTA	2947	CG2	THR	В	57	34.434	74.796	-18.685	1.00	34.17
30	MOTA	2948	С	THR	В	57	34.665	77.545	-17.667	1.00	38.22
	MOTA	2949	0	THR	В	57	34.196	77.556	-16.529	1.00	38.82
	MOTA	2950	N	ASP	В	58	34.117	78.198	-18.691	1.00	38.92
	MOTA	2951	CA	ASP	В	58	32.898	78.991	-18.557	1.00	38.50
	ATOM	2952	CB	ASP	В	58	31.737	78.118	-18.060	1.00	40.09
35	MOTA	2953	CG	ASP	В	58	31.472	76.911	-18.950	1.00	41.34

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	ATOM	2954	OD1	ASP	В	58	30.854	75.941	-18.464	1.00	42.69
	ATOM	2955	OD2	ASP	В	58	31.878	76.934	-20.133	1.00	43.89
	MOTA	2956	С	ASP	В	58	33.100	80.211	-17.660	1.00	38.07
	ATOM	2957	0	ASP	В	58	32.332	-80.445	-16.729	1.00	39.03
5	MOTA	2958	N	THR	В	59	34.137	80.984	-17.960	1.00	38.28
	MOTA	2959	CA	THR	В	59	34.465	82.187	-17.209	1.00	39.15
	MOTA	2960	СВ	THR	В	59	35.838	82.701	-17.622	1.00	38.09
	MOTA	2961	OG1	THR	В	59	36.825	81.710·	-17.404	1.00	38.32
	MOTA	2962	CG2	THR	В	59	36.263	83.960	-16.897	1.00	40.41
10	ATOM	2963	С	THR	В	59	33.401	83.263	-17.411	1.00	40.95
	ATOM	2964	0	THR	В	59	32.946	83.499	-18.535	1.00	43.05
	ATOM	2965	N	LYS	В	60	32.988	83.897	-16.315	1.00	41.08
	MOTA	2966	CA	LYS	В	60	31.949	84.922	-16.372	1.00	39.78
	ATOM	2967	CB	LYS	В	60	30.588	84.226	-16.264	1.00	39.82
15	ATOM	2968	CG	LYS	В	60	29.422	85.144	-15.953	1.00	40.01
	ATOM	2969	CD	LYS	В	60 .	28.092	84.454	-16.237	1.00	40.00
	ATOM	2970	CE	LYS	В	60	27.314	84.172	-14.961	1.00	40.98
	MOTA	2971	NZ	LYS	В	60	26.271	85.203	-14.710	1.00	42.05
	ATOM	2972	С	LYS	В	60	32.121	85.947	-15.255	1.00	39.73
20	ATOM	2973	0	LYS	В	60	32.221	85.585	-14.083	1.00	40.11
	ATOM	2974	N	VAL	В	61	32.146	87.229	-15.621	1.00	39.35
	ATOM	2975	CA	VAL	B	61	32.297	88.292	-14.631	1.00	37.83
•	ATOM	2976	. CB	VAL	В	61 ·	32.684	89.640	-15.272	1.00	37.73
	ATOM	2977	CG1	VAL	В	61	32.348	90.802	-14.347	1.00	37.25
25	ATOM	2978	CG2	VAL	В	61	34.167	89.649	-15.620	1.00	36.79
	MOTA	2979	С	VAL	В	61	31.025	88.442	-13.805	1.00	37.38
	ATOM	2980	0	VAL	В	61	29.979	88.845	-14.320	1.00	36.86
	MOTA	2981	N.	ILE	В	62	31.126	88.100	-12.524	1.00	35.32
	ATOM	2982	CA	ILE	B	62	29.993	88.177	-11.613	1.00	33.49
30	ATOM	2983	CB	ILE	B	62	29.849	86.898	-10.774	1.00	34.06
	MOTA	2984	CG2	LLE	В	62	29.257	85.777	-11.616	1.00	33.69
	MOTA	2985	CG:	LILE	ЕВ	62	31.200	86.490	-10.183	1.00	32.38
	MOTA	2986	CD	LILE	ВВ	62	31.092	85.548	-9.009	1.00	31.62
	MOTA	2987	С	ILI	В	62	30.070	89.381	-10.676	1.00	31.70
35	ATOM	2988	0	IL	E B	62 ·	29.042	89.855	-10.203	1.00	32.94

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	ATOM	2989	N	GLY		63	31.279		-10.400	1.00	
	ATOM	2990		GLY		63	31.414	91.001	-9.505	1.00	
	ATOM	2991	С	GLY		63	32.670	91.809	-9.732	1.00	
_	ATOM	2992	0	GLY	_	63	33.393		-10.708	1.00	
5	MOTA	2993	N	ASN			32.927	92.756	-8.827	1.00	
	MOTA	2994	CA	ASN	•	64	34.103	93.619	-8.924	1.00	
	MOTA	2995	CB	ASN	В	64	34.065		-10.203	1.00	
	MOTA	2996	CG	ASN	В	64	33.188	95.722	-10.099		34.17
	AŢOM	2997	OD1	ASN	В	64	32.086	95.689	-9.543	1.00	35.90
10	MOTA	2998	ND2	ASN	В	64	33.674	96.828	-10.646	1.00	34.72
	ATOM	2999	C	ASN	В	64	34.282	94.489	-7.681	1.00	30.61
	MOTA	3000	0	ASN	В	64	33.497	94.413	-6.738	1.00	31.75
	MOTA	3001	N	GLY	В	65	35.328	95.309	-7.694	1.00	29.88
	MOTA	3002	CA	GLY	B	65	35.617	96.185	-6.578	1.00	28.45
15	ATOM	3003	C	GLY	В	65 [.]	36.936	96.903	-6.745	1.00	28.07
	MOTA	3004	0	GLY	В	65	37.622	96.729	-7.748	1.00	29.15
	ATOM	3005	N	SER	В	66	37.287	97.708	-5.755	1.00	27.55
	MOTA	3006	CA	SER	В	66	38.531	98.481	-5.747	1.00	26.86
	MOTA	3007	СВ	SER	В	66	38.573	99.363	-4.498	1.00	31.61
20	ATOM	3008	OG	SER	В	66	38.374	98.581	-3.325	1.00	36.30
	MOTA	3009	С	SER	В	66	39.763	97.584	-5.766	1.00	26.13
	ATOM	3010	0	SER	В	66	40.881	98.061	-5.979	1.00	26.30
	MOTA	3011	N	PHE	В	67	39.551	96.290	-5.538	1.00	24.20
	MOTA	3012	CA	PHE	В	67	40.625	95.303	-5.526	1.00	23.70
25	MOTA	3013	CB	PHE	В	67	40.308	94.201	-4.519	1.00	19.77
	MOTA	3014	CG	PHE	В	67	39.001	93.542	-4.787	1.00	21.78
	ATOM	3015	CD1	PHE	В	67	37.892	93.860	-4.036	1.00	19.62
	ATOM	3016	CD2	PHE	В	67	38.875	92.622	-5.816	1.00	22.71
	ATOM	3017	CE1	PHE	В	67	36.676	93.276	-4.297	1.00	20.09
30	ATOM	3018	CE2	2 PHE	В	67	37.662	92.029	-6.084	1.00	21.51
	MOTA	3019	CZ	PHE	ВВ	67	36.558	92.359	-5.322	1.00	23.29
	MOTA	3020	C	PHE	ЕВ	67	40.827	94.686	-6.917	1.00	25.04
	ATOM	3021	0	PHI	ΣВ	67	41.933	94.267	-7.250	1.00	25.12
	ATOM	3022	N	GL	Y B	68	39.749	94.643	3 -7.724	1.00	27.00
3 <i>5</i> ·	MOTA	3023	CA	GL	Y B	68	39.842	94.097	-9.070	1.00	25.19

	ATOM	3024	С	GLY	В	68	38.965	92.885	-9.349	1.00	25.52
	ATOM	3025	0	GLY	В	68	39.227	91.803	-8.847	1.00	29.19
	ATOM	3026	N	VAL	В	69	37.969	93.092	-10.211	1.00	25.48
	MOTA	3027	CA	VAL	В	69	36.987	92.107	-10.735	1.00	23.30
5	ATOM	3028	CB	VAL	В	69	37.163	91.960	-12.266	1.00	24.41
	MOTA	3029	CG1	VAL	В	69	36.106	91.032	-12.863	1.00	21.84
	MOTA	3030	CG2	VAL	В	69	37.125	93.329	-12.934	1.00	25.19
	MOTA	3031	С	VAL	В	69	36.976	90.698	-10.128	1.00	2200
	ATOM	3032	0	VAL	В	69	38.003	90.099	-9.872	1.00	21.55
10	ATOM	3033	N	VAL	В	70	35.768	90.154	-9.986	1.00	22.14
	ATOM	3034	CA	VAL	В	70	35.551	88.799	-9.489	1.00	24.12
	MOTA	3035	CB	VAL	В	70	34.625	88.783	-8.250	1.00	24.16
•	MOTA	3036	CG1	VAL	В	70	34.275	87.355	-7.860	1.00	22.28
	MOTA	3037	CG2	VAL	В	70	35.280	89.508	-7.087	1.00	24.57
15	ATOM	3038	С	VAL	B	70	34.906	87.961	-10.582	1.00	26.12
	ATOM	3039	0	VAL	В	70	33.887	88.354	-11.143	1.00	27.62
	ATOM	3040	N	TYR	В	71	35.508	86.821	-10.891	1.00	28.54
	ATOM	3041	CA	TYR	В	71	34.993	85.953	-11.941	1.00	30.91
	ATOM	3042	СВ	TYR	В	71	36.127	85.503	-12.868	1.00	32.02
20	ATOM	3043	CG	TYR	В	71	36.962	86.617	-13.438	1.00	33.80
	ATOM	3044	CD1	TYR	В	71	36.682	87.152	-14.692	1.00	35.50
	ATOM	3045	CE1	TYR	В	71	37.458	88.166	-15.224	1.00	35.76
	ATOM	3046	CD2	TYR	В	71	38.040	87.128	-12.731	1.00	33.91
	ATOM	3047	CE2	TYR	В	71	38.820	88.144	-13.251	1.00	36.55
25	ATOM	3048	CZ	TYR	В	71	38.526	88.659	-14.499	1.00	36.56
	ATOM	3049	ОН	TYR	В	71	39.302	89.670	-15.021	1.00	36.97
	ATOM	3050	С	TYR	В	71	34.308	84.712	-11.409	1.00	31.87
	MOTA	3051	0	TYR	В	71	34.533	84.288	-10.281	1.00	33.24
	ATOM	3052	N	GLN	В	72	33.521	84.102	-12.278	1.00	32.22
30	MOTA	3053	CA	GLN	В	72	32.840	82.853	-11.989	1.00	33.30
	ATOM	3054	CB	GLN	В	72	31.331	82.971	-12.182	1.00	34.02
	ATOM	3055	CG	GLN	В	72	30.578	81.698	-11.824	1.00	36.90
	ATOM	3056	CD	GLN	В	72	29.132	81.713	-12.278	1.00	39.86
	ATOM	3057	OE1	GLN	В	72	28.226	81.366	-11.518	1.00	40.64
35	ATOM	3058	NE2	GLN	В	72	28.907	82.110	-13.526	1.00	41.43

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	MOTA	3059	С	GLN I	В	72	33.414	81.805	-12.935	1.00	34.05
•	MOTA	3060	0	GLN I	В	72	34.009	82.152	-13.957	1.00	35.56
	MOTA	3061	N	ALA	В	73	33.268	80.541	-12.600	1.00	33.40
	MOTA	3062	CA	ALA I	В	73	33.809	79.497	-13.447	1.00	33.76
5	MOTA	3063	СВ	ALA	В	73	35.322	79.590	-13.514	1.00	33.45
	MOTA	3064	С	ALA	В	73	33.376	78.131	-12.976	1.00	34.42
	ATOM	3065	0	ALA	В	73	32.735	77.995	-11.940	1.00	35.38
	MOTA	3066	N	LYS	В	74	33.720	77.123	-13.758	1.00	35.98
	ATOM	3067	CA	LYS	B	74	33.357	75.754	-13.445	1.00	36.46
10	ATOM	3068	CB	LYS	В	74	32.283	75.279	-14.435	1.00	38.65
	ATOM	3069	CG	LYS	В	74	31.862	73.821	-14.272	1.00	41.25
	ATOM	3070	CD	LYS	В	74.	30.968	73.360	-15.422	1.00	42.84
	MOTA	3071	CE	LYS	В	74	29.534	73.854	-15.259	1.00	45.68
-	MOTA	3072	NZ	LYS	В	74	28.787	73.877	-16.561	1.00	49.00
15	ATOM	3073	C	LYS	В	74	34.579	74.854	-13.505	1.00	36.82
	MOTA	3074	0	LYS	В	74	35.262	74.798	-14.531	1.00	36.80
	ATOM	3075	N	LEU	В	75	34.841	74.141	-12.406	1.00	36.09
	MOTA	3076	CA	LEU	В	75	35.970	73.220	-12.354	1.00	36.88
	MOTA	3077	CB	LEU	B _.	75	36.156	72.640	-10.944	1.00	34.57
20 ·	ATOM	3078	CG	LEU	В	75	36.267	73.649	-9.794	1.00	33.76
	ATOM	3079	CD1	LEU	В	75	36.456	72.925	-8.468	1.00	32.85
	ATOM	3080	CD2	LEU	В	75	37.403	74.635	-10.039	1.00	30.51
	MOTA	3081	С	LEU	В	75	35.725	72.102	-13.360	1.00	38.27
	MOTA	3082	Ο.	LEU	В	75	34.668	71.473	-13.355	1.00	36.48
25	MOTA	3083	N	CYS	В	76	36.680	71.891	-14.253	1.00	40.83
	ATOM	3084	CA	CYS	B	76	36.536	70.879	-15.292	1.00	43.19
	ATOM	3085	CB	CYS	В	76	37.699	70.935	-16.276	1.00	42.51
	MOTA	3086	SG	CYS	В	76	37.745	72.478	-17.226	1.00	42.48
	ATOM	3087	C,	· CYS	В	76	36.301	69.480	-14.730	1.00	45.58
30	MOTA	3088	0	CYS	В	76	35.391	68.777	-15.177	1.00	46.73
	MOTA	3089	N	ASP	В	77.	37.101	69.088	-13.735	1.00	48.25
	MOTA	3090	CA	ASP	В	77	36.957	67.775	-13.097	1.00	49.99
	MOTA	3091	CB	ASP	В	77	38.021	67.589	-12.004	1.00	52.61
	ATOM	3092	CG	ASP	В	77	38.090	68.757	-11.026	1.00	55.04
35	MOTA	3093	OD:	1 ASF	В	77	37.638	68.587	-9.868	1.00	56.33

	MOTA	3094	OD2	ASP	В	77	38.597	69.840	-11.418	1.00	55.51
	MOTA	3095	С	ASP	В	77	35.550	67.633	-12.513	1.00	50.49
	MOTA	3096	0	ASP	В	77	34.689	66.968	-13.092	1.00	51.15
	ATOM	3097	N	SER	В	78	35.316	68.306	-11.389	1.00	49.73
5	ATOM	3098	CA	SER	В.	78	34.013	68.317	-10.738	1.00	49.21
	MOTA	3099	СВ	SER	В	78 ·	34.181	68.391	-9.218	1.00	49.35
	ATOM	3100	OG	SER	В	78	35.081	69.425	-8.853	1.00	48.54
	ATOM	3101	С	SER	В	78	33.268	69.546	-11.231	1.00	48.71
	ATOM	3102	0	SER	В	78	33.792	70.651	-11.133	1.00	50.88
10	ATOM	3103	N	GLY	В	79	32.077	69.354	-11.794	1.00	46.72
	ATOM	3104	CA	GLY	В	79	31.309	70.471	-12.337	1.00	44.51
	ATOM	3105	С	GLY	В	79	31.000	71.572	-11.340	1.00	43.20
	ATOM	3106	0	GLY	В	79	30.140	72.418	-11.595	1.00	43.40
	ATOM	3107	N	GLU	В	80	31.691	71.563	-10.207	1.00	42.11
15	ATOM	3108	CA	GLU	В	80 .	31.487	72.557	-9.166	1.00	41.04
	ATOM	3109	CB	GLU	В	80	32.315	72.217	-7.922	1.00	41.90
	ATOM	3110	CG	GLU	В	80	31.699	71.145	-7.036	1.00	45.04
	ATOM	3111	CD	GLU	В	80	32.561	70.813	-5.831	1.00	47.24
	MOTA	3112	OE1	GLU	В	80	33.698	70.335	-6.029	1.00	48.62
20	MOTA	3113	OE2	GLU	В	80	32.107	71.049	-4.688	1.00	48.59
	MOTA	3114	С	GLU	В	80	31.800	73.970	-9.649	1.00	39.68
	ATOM	3115	0	GLU	В	80	32.860	74.236	-10.218	1.00	38.76
	ATOM	3116	N	LEU	В	81	30.873	74.875	-9.385	1.00	38.53
	MOTA	3117	CA	LEU	В	81	31.03Ò	76.278	-9.742	1.00	36.65
25	MOTA	3118	СВ	LEU	В	81	29.657	76.960	-9.771	1.00	37.93
	MOTA	3119	CG	LEU	В	81	28.814	76.770	-11.032	1.00	38.35
	ATOM	3120	CD1	LEU	В	81	27.597	75.903	-10.737	1.00	38.97
	ATOM	3121	CD2	LEU	В	81	28.388	78.122	-11.583	1.00	39.14
•	MOTA	3122	С	LEU	В	8 j	31.893	76.973	-8.693	1.00	35.35
30	ATOM	3123	0	LEU	В	81	31.798	76.669	-7.502	1.00	35.32
	ATOM	3124	N	VAL	В	82	32.714	77.914	-9.127	1.00	32.39
	ATOM	3125	CA	VAL	В	82	33.556	78.646	-8.206	1.00	29.03
	ATOM	3126	CB	VAL	В	82	34.971	78.024	-8.085	1.00	30.73
	MOTA	3127	CG1	VAL	В	82	34.905	76.603	-7.535	1.00	30.66
35	MOTA	3128	CG2	VAL	В	82	35.705	78.052	-9.421	1.00	32.95

	MOTA	3129	С	VAL E	3	82	33.699	80.101	-8.626	1.00 2	8.50
	ATOM	3130	0	VAL · E	3	82	33.447	80.469	-9.783	1.00 2	27.83
	ATOM .	3131	·N	ALA E	3	83	34.159	80.915	-7.693	1.00 2	24.36
	ATOM	3132	CA	ALA E	3	83	34.415	82.306	-7.958	1.00 2	21.31
5	MOTA	3133	СВ	ALA F	3	83	33.745	83.201	-6.929	1.00 2	22.68
	ATOM	3134	С	ALA I	3 _.	83	35.915	82.501	-7.956	1.00 2	21.78
	MOTA	3135	0	ALA I	3	83	36.647	81.684	-7.407	1.00 2	26.14
	ATOM	3136	N	ILE I	В	84	36.377	83.558	-8.578	1.00 2	21.94
	MOTA	3137	CA	ILE J	В	84	37.798	83.847	-8.643	1.00	21.77
10	ATOM	3138	CB	ILE !	В	84	38.433	83.419	-9.987	1.00	22.25
	ATOM	3139	CG2	ILE	В	84	39.949	83.531	-9.910	1.00	18.77
	ATOM	3140	CG1	ILE	B	84	38.002	81.993	-10.360	1.00	18.57
	ATOM	3141	CD1	IĻE	В	84	39.021	81.226	-11.176	1.00	21.85
	MOTA	3142	С	ILE	В	84	37.973	85.323	-8.450	1.00	24.02
15	ATOM	3143	0	ILE	В	84	37.587	86.101	-9.317	1.00	25.19
	ATOM	3144	N	LYS	В	85	38.502	85.699	-7.283	1.00	25.57
	ATOM	3145	CA	LYS	В	85	38.682	87.102	-6.923	1.00	26.87
	ATOM	3146	CB	LYS	В	85	39.024	87.238	-5.433	1.00	27.80
	ATOM	3147	CG	LYS	В	85	38.917	88.654	-4.919	1.00	27.48
20	ATOM .	3148	CD	LYS	В	85	38,186	88.713	-3.585	1.00	28.88
	MOTA	3149	CE	LYS	В	85	38.215	90.121	-3.004	1.00	29.25
	MOTA	3150	NZ.	LYS	В	85	37.788	90.150	-1.571	1.00	31.82
	MOTA	3151	С	LYS	В	85	39.732	87.817	-7.777	1.00	28.36
	ATOM	3152	0	LYS	В	85_	39.404	88.764	-8.475	1.00	32.62
25	MOTA	3153	N	LYS	В	86	40.982	87.406	-7.725	1.00	27.30
	MOTA	3154	CA	LYS	В	86	42.012	88.079	-8.524	1.00	28.47
	MOTA	3155	СВ	LYS	В	86	41.647	88.040	-10.024	1.00	29.75
	MOTA	3156	CG	LYS	В	86	42.626	88.785	-10.918	1.00	30.30
	MOTA	3157	CD	LYS	В	86 .	42.448	88.399	-12.385	1.00	31.97
30	ATOM	3158	ÇE	LYS	В	86	43.646	88.817	-13.229	1.00	32.33
	MOTA	3159	NZ	LYS	В	86	43.528	90.223	-13.718	1.00	32.44
	ATOM	3160) C	LYS	В	86	42.191	89.526	-8.080	1.00	28.16
	ATOM	3161	L O	LYS	В	86	41.398	90.390	-8.426	1.00	27.79
	ATOM	3162	2 N	IAV	B د	87	43.237	89.787	-7.310	1.00	30.21
35	MOTA	3163	3 C <i>I</i>	IAV A	ЪВ	87	43.505	91.136	-6.818	1.00	31.57

	MOTA	3164	CB	VAL	В	87	43.348	91.245	-5.275	1.00	30.87
	ATOM	3165	CG1	VAL	В	87	42.229	90.345	-4.773	1.00	28.72
	ATOM	3166	CG2	VAL	В	87	44.652	.90.928	-4.564	1.00	30.54
	ATOM	3167	С	VAL	В	87	44.888	91.624	7.228	1.00	32.63
5	ATOM	3168	0	VAL	В	87	45.834	90.847	-7.301	1.00	32.63
	ATOM	3169	N	LEU	В	88	44.994	92.923	-7.479	1.00	36.02
	ATOM	3170	CA	LEU	В	88	46.258	93.530	-7.864	1.00	38.65
	ATOM	3171	CB	LEU	В	88	46.027	94.939	-8.428	1.00	38.60
	ATOM	3172	CG	LEU	В	88	46.980	95.389	-9.542	1.00	39.38
10	MOTA	3173	CD1	LEU	В	88	46.418	96.600	-10.274	1.00	39.21
	ATOM	3174	CD2	LEU	В	88	48.361	95.697	-8.981	1.00	38.72
	MOTA	3175	С	LEU	В	88	47.170	93.594	-6.654	1.00	41.80
	ATOM	3176	0	LEU	В	88	46.864	94.277	-5.672	1.00	43.27
	ATOM	3177	N	GLN	.B	89	48.277	92.867	-6.715	1.00	44.15
15	ATOM	3178	CA	GLN	В	89	49.223	92.830	-5.608	1.00	46.43
	MOTA	3179	СВ	GLN	В	89	49.313	91.407	-5.054	1.00	46.20
	ATOM	3180	CG	GLN	В	89	48.297	91.098	-3.973	1.00	47.54
	ATOM	3181	CD	GLN	В	89	48.617	91.789	-2.668	1.00	47.37
	ATOM	3182	OE1	GLN	В	89	47.905	92.700	-2.245	1.00	49.60
20	ATOM	3183	NE2	GLN	В	89	49.695	91.361	-2.022	1.00	49.76
	ATOM	3184	С	GLN	В	89	50.618	93.309	-6.009	1.00	48.98
	ATOM	3185	0	GLN	В	89	50.911	93.544	-7.187	1.00	49.03
	MOTA	3186	N	ASP	В	90	51.481	93.419	-5.008	1.00	50.77
	ATOM	3187	CA .	ASP	В	90	52.864	93.827	-5.202	1.00	52.86
25	ATOM	3188	СВ	ASP	В	90	53.067	95.278	-4.755	1.00	52.56
	ATOM	3189	CG	ASP	В	90	54.310	95.921	-5.352	1.00	52.43
•	ATOM	3190	OD1	ASP	В	90	54.173	96.967	-6.024	1.00	51.92
	ATOM	3191	OD2	ASP	В	90	55.421	95.385	-5.141	1.00	52.38
- :	ATOM	3192	С	ASP	В	90	53.777	92.891	-4.409	1.00	54.65
30	ATOM	3193	0	ASP	В	90	53.481	92.563	-3.252	1.00	55.24
	ATOM	3194	N	LYS	В	91	54.873	92.451	-5.039	1.00	55.69
	ATOM	3195	CA	LYS	В	91	55.824	91.507	-4.429	1.00	56.44
	ATOM	3196	CB	LYS	В	91	57.142	91.480	-5.177	1.00	56.74
-	ATOM	3197	CG	LYS	В	91	57.101	90.724	-6.482	1.00	56.89
35	MOTA	3198	CD	LYS	В	91	56.988	91.646	-7.701	1.00	56.85

•	MOTA	3199	CE	LYS E	3	91		58.103	91.365	-8.705	1.00	56.60
	ATOM	3200	NZ	LYS E	3	91		59.228	92.329	-8.574	1.00	54.94
	ATOM	3201	С	LYS E	3	91		56.118	91.932	-3.003	1.00	57.84
	ATOM	3202	0	LYS E	3	91		56.174	91.130 .	-2.073	1.00	57.47
5	MOTA	3203.	N	ARG F	3	92		56.293	93.242	-2.898	1.00	59.51
	ATOM	3204	CA	ARG E	3	92		56.440	93.812	-1.612	1.00	60.32
	ATOM	3205	CB	ARG I	3	92		56.567	95.344	-1.628	1.00	61.19
	ATOM	3206	CG	ARG I	3	92		55.223	96.051	-1.807	1.00	62.74
	MOTA	3207	CD.	ARG I	В	92		55.091	97.310	-0.936	1.00	64.16
10	MOTA	3208	NE	ARG 1	В	92		53.734	97.452	-0.383	1.00	64.89
	ATOM	3209	CZ	ARG	В	92		52.690	97.943	-1.040	1.00	65.15
	ATOM	3210	NH1	ARG	В	92	•	52.815	98.353	-2.303	1.00	64.76
	MOTA	3211	NH2	ARG :	В	92		51.510	98.013	-0.431	1.00	65.43
	MOTA	3212	C	ARG	В	92	•	55.257	93.328	-0.871	1.00	60.27
15	ATOM	3213	0	ARG	В	92		54.114	93.626	-1.167	1.00	60.72
	ATOM	3214	N	PHE	В	93		55.628	92.551	0.093	1.00	59.54
	MOTA	3215	CA	PHE	В	93		54.728	92.058	1.098	1.00	58.24
	MOTA	3216	CB	PHE	В	93		53.931	93.238	1.611	1.00	59.80
	MOTA	3217	CG	PHE	В	93		53.712	92.969	3.023	1.00	60.86
20	ATOM	3218	CD1	PHE	В	93		54.604	93.373	4.005	1.00	61.43
	ATOM	3219	CD2	PHE	В	93		52.576	92.292	3.388	1.00	61.79
	ATOM	3220	CE1	PHE	В	93		54.375	93.046	5.329	1.00	61.52
	ATOM	3221	CE2	PHE	В	93		52.334	91.959	4.705	1.00	61.96
	MOTA	3222	CZ	·PHE	В	93		53.237	92.338	5.680	1.00	62.16
25	MOTA	3223	. C	PHE	В	93		53.820	90.910	0.699	1.00	56.34
	ATOM	3224	0	PHE	В	93		53.778	90.473	-0.455	1.00	57.26
	ATOM	3225	N	LYS	В	94		53.119	90.395	1.720		52.33
	ATOM	3226	CA	LYS	В	94	ŕ	52.161	89.300	1.568		48.31
	ATOM	3227	CB	LYS	В	94		52.287	88.270	2.684	1.00	49.90
30	ATOM	3228	CG	LYS	В	94		53.621	87.546	2.734		52.02
	ATOM	3229	CD	LYS	В	94		53.888	86.960	4.100		53.08
	MOTA	3230	CE	LYS	В	94 .		53.772	88.029	5.182	1.00	54.32
	ATOM	3231	NZ	LYS	В	94		54.367	87.569	6.472		55.37
	ATOM	3232	С	LYS	В	94		50.758	89.872	1.626		44.39
35	MOTA	3233	0	LYS	В	94		50.553	90.937	2.204	1.00	45.14

	ATOM	3234	N	ASN	В	95	49.794	89.177	1.034	1.00	39.77
	ATOM	3235	ĊA	ASN	В	95	48.405	89.632	1.033	1.00	35.63
	MOTA	3236	CB	ASN	В	95	47.633	88.938 .	-0.097	1.00	32.69
	MOTA	3237	CG	ASN	B`	95 [°]	46.296	89.579	-0.405	1.00	30.84
5	ATOM	3238	OD1	ASN	В	95	46.226	90.620	-1.056	1.00	31.82
	ATOM	3239	ND2	ASN	В	95	45.223	88.948	0.074	1.00	30.54
	ATOM	3240	С	ASN	В	95 .	47.767	89.300	2.384	1.00	32.38
	ATOM	3241	0	ASN	В	95	47.910	88.186	2.870	1.00	32.37
	MOTA	3242	N	ARG	В	96	47.078	90.267	2.985	1.00	31.13
10	MOTA	3243	CA	ARG	В	96	46.436	90.058	4.287	1.00	27.36
	MOTA	3244	CB	ARG	В	96	45.985	91.396	4.889	1.00	27.69
	MOTA	3245	CG	ARG	В	96	45.479	91.288	6.331	1.00	28.43
	ATOM	3246	CD	ARG	В	96 .	46.149	92.303	7.239	1.00	29.78
	MOTA	3247	NE	ARG	В	96	45.441	93.580	7.248	1.00	30.41
15	ATOM	3248	CZ	ARG	В	96	45.959	94.720	7.709	1.00	30.73
	MOTA	3249	NH1	ARG	В	96 .	47.204	94.760	8.188	1.00	32.67
	ATOM	3250	NH2	ARG	В	96	45.229	95.827	7.690	1.00	31.28
	ATOM	3251	С	ARG	В	96	45.248	89.116	4.158	1.00	26.30
	MOTA	3252	0	ARG	B	96	45.040	88.237	4.995	1.00	24.70
20	MOTA	3253	N	GLU	В	97	44.466	89.298	3.098	1.00	24.76
	ATOM	3254	CÀ	GLU	В	97	43.303	88.458	2.867	1.00	22.51
	MOTA	3255	CB	GLU	В	97	42.435	89.003	1.733	1.00	24.93
	MOTA	3256	CG .	GLU	В	97	41.267	88.104	1.334	1:00	22.80
•	ATOM	3257	CD	GLU	В	97	40.263	88.812	0.447	1.00	21.64
25	MOTA	3258	OE1	GLU	В	97 ·	39.079	88.414	0.461	1.00	25.04
	ATOM	3259	OE2	GLU	В	97	40.655	89.772	-0.253	1.00	21.61
	MOTA	3260	С	GLU	В	97	43.686	87.009	2.621	1.00	21.52
	MOTA	3261	Ο.	GLU	В	97	42.930	86.109	2.985	1.00	24.82
	ATOM	3262	N	LEU	В	98	44.855	86.778	2.014	1.00	19.37
30	ATOM	3263	CA	LEU	В	98	45.308	85.413	1.740	1.00	18.57
	MOTA	3264	CB	LEU	В	98	46.387	85.371	0.664	1.00	16.63
	MOTA	3265	CG	LEU	В	98	46.977	83.985	0.367	1.00	16.92
	ATOM	3266	CD1	LEU	В	98 .	45.897	83.012	-0.077	1.00	13.54
	MOTA	3267	CD2	LEU	В	98	48.094	84.072	-0.672	1.00	18.79
35	ATOM	3268	С	LEU	В	98	45.811	84.700	3.000	1.00	18.68

	ATOM	3269	0	LEU B	98	45.533	83.525	3.194	1.00 15.55
	ATOM	3270	N	GLN B	99	46.560	85.411	3.835	1.00 19.69
	ATOM	3271	CA	GLN B	99	47.084	84.812	5.058	1.00 23.79
	ATOM	3272	СВ	GLN B	99	48.052	85.757 .	5.787	1.00 27.75
5	MOTA	3273	CG	GLN B	99	49.373	85.988	5.059	1.00 33.53
	ATOM	3274	CD	GLN B	99	50.471	84.998	5.447	1.00 38.62
	MOTA	3275	OE1	GLN B	99	51.624	85.384	5.657	1.00 39.28
	ATOM	3276	NE2	GLN B	99	50.124	83.711	5.532	1.00 41.46
	ATOM	3277	С	GLN B	99	45.934	84.387	5.965	1.00 19.19
10	ATOM	3278	0	GLN B	99	45.941	83.297	6.508	1.00 19.09
	MOTA	3279	N	ILE B	100 .	44.934	85.244	6.074	1.00 19.23
	MOTA	3280	CA	ILE B	100	43.747	84.962	6.876	1.00 20.77
	ATOM	3281	CB	ILE B	100	42.864	86.221	7.025	1.00 18.98
	MOTA	3282	CG2	ILE B	100	41.433	85.860	7.381	1.00 18.23
15	ATOM	3283	CG1	ILE B	100	43.461	87.169	8.068	1.00 17.33
	ATOM	3284	CD1	ILE B	100	42.907	88.570	8.006	1.00 12.19
	MOTA	3285	С	ILE B	100	42.921	83.796	6.314	1.00 23.82
	MOTA	3286	0	ILE B	100	42.554	82.875	7.045	1.00 24.69
	ATOM	3287	N	MET B	101	42.618	83.839	5.017	1.00 24.18
20	MOTA	3288	CA	MET B	101	41.821	82.786	4.379	1.00 24.19
	ATOM	3289	СВ	MET B	101	41.449	83.182	2.953	1.00 26.26
	MOTA	3290	CG	MET B	101	40.491	84.346	2.889	1.00 28.56
•	ATOM	3291	SD	MET E	3 101	39.096	84.023	1.802	1.00 37.47
	ATOM	3292	CE	MET E	3 101	39.857	84.336	0.207	1.00 35.49
25	ATOM	3293	С	MET E	3 101	42.497	81.418	4.392	1.00 22.54
	ATOM	3294	· O	MET I	3 101	41.820	80.400	4.397	1.00 23.04
	ATOM	. 3295	N	ARG I	3 102	43.826	81.402	4.391	1.00 23.08
	ATOM	3296	CA	ARG I	B 102	44.595	80.157	4.393	1.00 25.61
	MOTA	3297	ÇE	ARG 1	в 102	46.081	80.464	4.248	1.00 26.73
30	MOTA	3298	3 CG	ARG	B 102	46.515	80.714	2.808	
	ATOM	3299	e C	ARG,	B 102	47.209	79.504	2.214	1.00 29.82
	MOTA	3300	N C	E ARG	B 102	48.581	T9.809	1.828	1.00 32.54
	MOTA	330	1 C	Z ARG	В 102	49.489	78.884	1.525	
	MOTA	330	2 NI	H1 ARG	В 102	49.19			
35	MOTA	330	3 N	H2 ARG	B 102 ⁻	50.699	9 79.255	1.116	1.00 34.43

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	ATOM	3304	С	ARG	В	102	44.382	79.304	5.653	1.00	27.37
	MOTA	3305	0	ARG	В	102	44.565	78.085	5.610	1.00	26.87
	MOTA	3306	N	LYS	В	103	44.025	79.921	6.783	1.00	27.22
•	MOTA	3307	CA	LYS	В	103	43.846	79.138 .	8.011	1.00	27.60
5	ATOM	3308	CB	LYS	В	103	44.393	79.896	9.241	1.00	27.93
	MOTA	3309	CG	LYS	В	103	43.938	81.334	9.368	1.00	27.88
	ATOM	3310	CD	LYS'	В	103	45.024	82.193	9.987	1.00	31.30
	ATOM	3311	CE	LYS	В	103	44.914	82.226	11.511	1.00	31.30
	MOTA	3312	NZ	LYS	В	103	45.771	83.294	12.115	1.00	31.93
10	ATOM	3313	C	LYS	В	103	42.398	78.698	8.240	1.00	25.91
	MOTA	3314	0	LYS	В	103	42.151	77.778	9.016	1.00	28.69
	MOTA	3315	N	LEU	В	104 .	41.443	79.348	7.585	1.00	25.04
	MOTA	3316	CA	LEU	В	104	40.035	79.010	7.775	1.00	24.60
	ATOM	3317	CB	LEU	В	104	39.145	80.195	7.467	1.00	24.10
15	ATOM	3318	CG	LEU	В	104	39.554	81.518	8.097	1.00	25.73
	ATOM	3319	CD1	LEU	В	104	38.566	82.615	7.698	1.00	22.14
	MOTA	3320	CD2	LEU	В	104	39.648	81.378	9.620	1.00	24.52
	ATOM	3321	С	LEU	B·	104	39.533	77.774	7.026	1.00	26.61
	MOTA	3322	0	LEU	В	104	39.899	77.505	5.872	1.00	27.07
20	ATOM	3323	N	ASP	В	105	38.639	77.061	7.701	1.00	23.86
	ATOM	3324	CA	ASP	В	105	37.980	75.877	7.182	1.00	24.16
	MOTA	3325	CB	ASP	В	105	38.895	74.644	7.229	1.00	25.34
	ATOM .	3326	CG	ASP	В	105	38.388	73.488	6.369	1.00	27.01
	MOTA	3327	OD1	ASP	В	105	37.178	73.457	6.045	1.00	27.72
25	ATOM	3328	OD2	ASP	В	105	39.204	72.611	6.017	1.00	31.45
	MOTA	3329	С	ASP	В	105	36.716	75.644	7.990	1.00	22.82
	ATOM	3330	0	ASP	В	105	36.706	74.842	8.904	1.00	24.78
	ATOM	3331	N	HIS	В	106	35.667	76.395	7.670	1.00	23.73
	ATOM	3332	CA	HIS	В	106	34.410	76.312	8.391	1.00	24.16
30	MOTA	3333	CB	HIS	Ŗ	106	34.305	77.498	9.376	1.00	26.05
	ATOM	3334	CG	HIS	В	106	33.192	77.392	10.378	1.00	24.58
	ATOM	3335	CD2	HIS	В	106	33.198	76.989	11.672	1.00	24.11
	MOTA	3336	ND1	HIS	В	106	31.887	77.723	10.089	1.00	24.83
	ATOM	3337	CE1	HIS	В	106	31.138	77.526	11.157	1.00	25.65
`35	ATOM	3338	NE2	HIS	В	106	31.912	77.080	12.129	1.00	21.29

	ATOM	3339	С	HIS	В	106	33.1	199	76.260	7.4	61	1.00	23.88
	ATOM	3340	0	HIS	В	106	33.1	111	77.000	6.4	75	1.00	25.00
	ATOM	3341	N	CYS	В	107	32.2	269	75.374	7.8	03	1.00	24.06
	ATOM	3342	CA	CYS	В	107	31.0	027	75.144	7.0	63	1.00	25.46
5 *	ATOM	3343	CB '	CYS	В	107	30.1	192	74.052	7.7	4.4	1.00	28.48
	ATOM	3344	SG	CYS	В	107	29.3	366	74.561	9.2	85	1.00	32.88
	ATOM	3345	С	CYS	В	107	.30.3	178	76.393	6.8	56	1.00	25.19
	ATOM	3346	0	CYS	В.	107	29.2	239	76.365	6.0	57	1.00	25.17
	ATOM	3347	N	ASN	В	108	30.4	485	77.486	7.5	69	1.00	23.81
10	MOTA	3348	CA	ASN	В	108	29.7	705	78.721	7.4	24	1.00	21.66
	MOTA	3349	CB	ASN	В	108	29.0	032	79.128	8.7	4б	1.00	24.36
	MOTA	3350	CG	ASN	В	108	27.8	872	78.227	9.1	27	1.00	24.89
	ATOM	3351	OD1	ASN	В	108	27.8	861	77.637	10.2	13	1.00	26.27
	MOTA	3352	ND2	ASN	В	108	26.	883	78.117	8.2	42	1.00	25.27
15	ATOM	3353	C	ASN	В	108	30.	559	79.865	6.9	01	1.00	20.89
	MOTA	3354	Ο.	ASN	B _.	108	30.	1,71	81.034	6.9	93	1.00	20.76
	ATOM	3355	N	ILE	В	109	31.	716	79.520	6.3	51	1.00	19.97
	ATOM	3356	CA	ILE	В	109	32.	635	80.493	5.7	96	1.00	19.68
	ATOM	3357	CB	ILE	В	109	33.	913	80.592	6.6	46	1.00	18.06
20	MOTA	3358	CG2	ILE	В	109	34.	908	81.558	6.0	16	1.00	16.00
	MOTA	3359	CG1	ILE	В	109	33.	592	81.001	8.1	00 ,	1.00	18.80
	ATOM	3360	CD1	ILE	В	109	34.	831	81.254	8 [.] . 9	24	1.00	13.72
•	ATOM	3361	С	ILE	В	109	33.	032	80.077	4.3	64	1.00	21.70
	MOTA	3362	0	ILE	В	109	33.	433	78.930	4.1	.30	1.00	20.77
25	MOTA	3363	N	VAL	В	110	32.	940	81.012	3.4	19	1.00	21.55
•	MOTA	3364	CA	VAL	В	110	33.	32.0	80.709	2.0	41	1.00	21.63
	MOTA	3365	CB	LAV	В	110	33.	105	81.906	1.1	.05	1.00	22.38
	MOTA	3366	CG1	VAL	В	110	34.	312	82.830	1.1	.05	1.00	22.92
•	ATOM	3367	CG2	VAL	В	110	32.	790	81.412	-0.3	300	1.00	27.31
30	ATOM	3368	С	VAL	В	110	34.	763	80.225	2.0	001	1.00	20.46
	MOTA	3369	0	VAL	В	110	35.	683	80.934	2.3	375	1.00	22.12
	MOTA	3370	N	ARG	В	111	34.	947	78.991	1.6	505	1.00	20.95
	MOTA	3371	CA	ARG	В	111	36.	275	78.392	1.5	583	1.00	23.52
	ATOM	3372	. CB	ARG	В	111	36.	131	76.870	1.5	528	1.00	25.99
35	MOTA	3373	CG	ARG	B	111	37.	. 383	76.111	1.9	916	1.00	31.22

	ATOM	3374	CD	ARG B	111	37.135	74.610	1.908	1.00 35.06
	ATOM	3375	NE	ARG B	111	38.031	73.906	0.984	1.00 39.62
	ATOM	3376	CZ	ARG B	111	37.618	73.149	-0.040	1.00 41.78
	ATOM	3377	NHl	ARG B	111	36.316	73.020	-0.324	1.00 42.77
5	ATOM	3378	NH2	ARG B	111	38.518	72.522	-0.790	1.00 42.63
	ATOM	3379	С	ARG B	111	37.144	78.871	0.410	1.00 24.24
	ATOM	3380	0	ARG B	111	36.639	79.231	-0.652	1.00 25.26
	ATOM	3381	N	LEU B	112	38.460	78.809	0.623	1.00 22.36
	ATOM	3382	CA	LEU B	112	39.462	79.149	-0.373	1.00 22.52
10	ATOM	3383	СВ	LEU B	112	40.598	79.988	0.223	1.00 21.19
	ATOM	3384	CG	LEU B	112	41.887	80.060	-0.609	1.00 22.47
	MOTA	3385	CD1	LEU B	112	41.740	81.070	-1.738	1.00 21.76
	ATOM	3386	CD2	LEU B	112	43.085	80.407	0.265	1.00 22.74
	ATOM	3387	С	LEU B	112	40.020	77.841	-0.906	1.00 22.82
15	ATOM	3388	0	LEU B	112	40.875	77.221	-0.274	1.00 23.51
	ATOM	3389	N	ARG B	113	39.493	77.410	-2.051	1.00 22.73
	ATOM	3390	CA	ARG B	113	39.898	76.151	-2.682	1.00 21.00
٠	ATOM	3391	CB	ARG B	113	39.011	75.873	-3.882	1.00 23.79
	ATOM	3392	CG	ARG B	113	37.537	75.936	-3.562	1.00 22.88
20	ATOM	3393	CD	ARG B	113	36.966	74.547	-3.378	1.00 29.46
	ATOM	3394	NE	ARG B	113	35.586	74.464	-3.842	1.00 31.60
	ATOM	3395	CZ	ARG B	113	35.139	73.536	-4.679	1.00 30.00
	MOTA	3396	NHl	ARG B	113	35.958	72.627	-5.197	1.00 31.17
	ATOM	3397	NH2	ARG B	113	33.865	73.528	-5.005	1.00 34.17
25	MOTA	3398	С	ARG B	113	41.335	76.192	-3.134	1.00 18.67
	ATOM	3399	0	ARG B	113	42.112	75.277	-2.876	1.00 19.77
	ATOM	3400	N	TYR B	114	41.681	77.250	-3.828	1.00 19.73
	ATOM	3401	CA	TYR B	114	43.031	77.415	-4.334	1.00 17.83
	MOTA	3402	СВ	TYR B	114	43.184	76.791	-5.736	1.00 18.92
. 30	MOTA	3403	CG	TYR B	114	42.707	75.373	-5.904	1.00 15.37
	ATOM	3404	CD1	TYR B	114	41.386	75.104	-6.166	1.00 17.28
	ATOM	3405	CE1	TYR B	114	40.948	73.811	-6.347	1.00 19.97
	ATOM	3406	CD2	TYR B	114	43.591	74.312	-5.825	1.00 17.10
	ATOM	3407	CE2	TYR B	114	43.162	73.019	-6.000	1.00 18.35
35	ATOM	3408	CZ	TYR B	114	41.841	72.777	-6.263	1.00 19.67

		2400	011	m v.D	D	111	47 404	71.490	-6.446	1.00	26 72
	ATOM	3409	OH	TYR			41.404			1.00	
	ATOM	3410	C			114	43.344	78.875	-4.473		
	MOTA	3411	0			114	42.468	79.707	-4.467	1.00	
_	MOTA	3,412	N			115	44.597	79.163		1.00	
5	ATOM	3413	CA			115	45.039	80.510	-4.890	1.00	
	ATOM	3414	CB			115	45.399	81.242	-3.594		18.79
	MOTA	3415	CG			115	46.608	80.724	-2.891		17.82
	MOTA	3416	CD1	PHE	В	115	47.845	81.278	-3.127		17.38
	MOTA	3417	CD2	PHE	В	115	46.498	79.690	-1.978		21.19
10	ATOM	3418	CE1	PHE	В	115	48.966	80.813	-2.468	1.00	21.69
	MOTA	3419	CE2	PHE	В	115	47.613	79.214	-1.311	1.00	22.13
	MOTA	3420	CZ	PHE	В	115	48.852	79.777	-1.556	1.00	21.81
	ATOM	3421	C	PHE	В	115	46.206	80.448	-5.833	1.00	20.99
	MOTA	3422	0	PHE	В	115	46.956	79.495	-5.806	1.00	21.58
15	MOTA	3423	N	PHE	В	116	46.365	81.441	-6.668	1.00	23.42
	ATOM	3424	CA	PHE	В	116	47.487	81.423	-7.589	1.00	23.63
	ATOM	3425	СВ	PHE	В	116	47.263	80.485	-8.785	1.00	24.34
	MOTA	3426	CG	PHE	В	116	46.116	80.843	-9.690	1.00	23.63
	MOTA	3427	CD1	PHE	B	116	46.322	81.640	-10.808	1.00	23.38
20	MOTA	3428	CD2	PHE	B	116	44.847	80.366	-9.435	1.00	21.16
	ATOM	3429	CE1	PHE	E	116	45.270	81.952	-11.653	1.00	23.56
	ATOM	3430	CE2	PHE	: E	3 116	43.787	80.673	-10.269	1.00	24.99
	ATOM	3431	CZ	PHE	C E	3 116	43.998	81.469	-11.386	1.00	22.81
	ATOM	3432	С	PHI	E E	3 116	47.871	82.803	-8.025	1.00	24.48
25	ATOM	3433	0	PHI	E E	3 116	47.023	83.666	-8.224	1.00	25.63
	MOTA	3434	N	TYI	R I	3 117	49.158	83.001	-8.169	1.00	27.57
	ATOM	3435	CA	TY	R I	3 117	49.668	84.268	-8.592	1.00	30.79
	ATOM	3436	CB	TY!	R .I	3 117	50.979	84.558	-7.894	1.00	30.32
	AŢOM	3437	CG	TY:	Ŗ I	B 117	50.828	84.766	-6.409	1.00	31.52
30	ATOM	3438	CD:	l TY	R i	B 117	50.998	83.714	-5.525	1.00	32.20
	ATOM	3439	CE:	1 TY	R :	в 117	50.877	83.897	-4.162	1.00	33.83
	ATOM	3440	CD	2 TY	R	в 117	50.527	86.011	-5.892	1.00	31.27
	ATOM	3441	CE	2 TY	R	B 117	50.401	86.206	-4.526	1.00	34.81
	ATOM	3442	CZ	TY	R	В 117	50.579	85.142	-3.666	1.00	34.02
35	ATOM	3443		TY	R	B 117	50.464	85.328	-2.302	1.00	35.99

	ATOM	3444	С	TYR E	3	117	49.856	84.252	-10.096	1.00	33.65
	MOTA	3445	0	TYR E	3	117	50.534	83.379	-10.631	1.00	34.07
	MOTA	3446	N	SER E	3	118	49.242	85.216	-10.764	1.00	37.02
	MOTA	3447	CA	SER E	3	118	49.333	85.336	-12.208	1.00	39.81
5	MOTA	3448	CB	SER E	3	118	47.956	85.205	-12.857	1.00	38.58
	MOTA	3449	OG	SER E	3	118	47.192	86.387	-12.690	1.00	38.24
	ATOM	3450	C	SER E	3	118	49.957	86.667	-12.563	1.00	43.00
	MOTA	3451	0	SER E	3	118	49.586	87.701	-12.005	1.00	43.48
	MOTA	3452	N	SER E	3	119	50.909	86.638	-13.489	1.00	47.48
10	MOTA	3453	CA	SER E	3	119	51.593	87.851	-13.925	1.00	50.85
	ATOM	3454	CB,	SER E	3	119	52.586	87.527	-15.046	1.00	50.24
	MOTA	3455	OG	SER E	3	119	53.919	87.542	-14.571	1.00	50.41
	ATOM	3456	С	SER E	3	119	50.582	88.886	-14.412	1.00	53.19
	MOTA	3457	0	SER E	3	119	49.580	88.539	-15.046	1.00	54.05
15	ATOM	3458	N	GLY F	3	120	50.847	90.151	-14.114	1.00	55.50
	ATOM	3459	CA	GLY F	3	120	49.945	91.200	-14.543	1.00	59.54
	ATOM.	3460	C	GLY F	3	120	50.379	91.787	-15.869	1.00	62.44
	MOTA	3461	0	GLY E	3	120	50.860	91.067	-16.752	1.00	63.06
	ATOM	3462	N	GLU H	3	121	50.239	93.095	-16.006	1.00	64.20
20	ATOM	3463	CA	GLU H	3	121	50.649	93.770	-17.225	1.00	66.57
	ATOM	3464	CB	GLU I	3	121 .	49.755	94.988	-17.490	1.00	67.06
	MOTA	3465	CG	GLU I	В	121	48.261	94.741	-17.278	1.00	67.73
	MOTA	3466	CD	GLU I	В	121	47.817	93.328	-17.636	1.00	68.42
	MOTA	3467	OE1	GLU 1	В	121	47.922	92.945	-18.828	1.00	68.67
25	ATOM	3468	OE2	GLU I	В	121	47.359	92.604	-16.723	1.00	67.90
	ATOM	3469	С	GLU 1	В	121	52.115	94.176	-17.098	1.00	67.64
	ATOM	3470	0	GLU 1	В	121	52.472	95.334	-17.317	1.00	68.09
	ATOM	3471	N	LYS :	B-	122	52.952	93.198	-16.705	1.00	69.00
	ATOM	3472	CA	LYS	В	122	54.382	93.412	-16.491	1.00	69.57
30	ATOM	3473	CB	LYS	В	122	55.073	93.868	-17.792	1.00	70.71
	MOTA	3474	CG	LYS	В	122	55.288	92.745	-18.799	1.00	71.91
	ATOM	3475	CD	LYS	В	122	53.980	92.288	-19.436	1.00	72.78
	ATOM	3476	CE	LYS	В	122	53.547	90.925	-18.911	1.00	73.05
	ATOM	3477	NZ	LYS	В	122	52.474	90.319	-19.753	1.00	72.80
35	MOTA	3478	С	LYS	В	122	54.578	94.407	-15.328	1.00	.69.47

	ATOM	3479	0	LYS B	122	54.018	94.190	-14.248	1.00	70.33
	MOTA	3480	N	LYS B	123	55.351	95.490	-15.533	1.00	68.70
	ATOM	3481	CA	LYS B	123	55.584	96.491 ·	-14.479	1.00	67.63
	MOTA	3482	CB	LYS B	123	54.274	97.231	-14.124	1.00	67.63
5	MOTA	3483	CG	LYS B	123	53.129	97.002	-15.102	1.00	67.45
	ATOM	3484	CD	LYS B	123	52.314	98.268	-15.329	1.00	68.76
	ATOM	3485	CE	LYS B	123	52.831	99.071	-16.521	1.00	69.10
	ATOM	3486	NZ	LYS B	123	52.538	98.409	-17.828	1.00	68.94
	ATOM	3487	С	LYS B	123	56.173	95.834	-13.223	1.00	66.56
10	MOTA	3488	0	LYS B	123	56.777	94.759	-13.300	1.00	66.55
	MOTA	3489	N	ASP B	124	55.979	96.469	-12.065	1.00	65.01
	ATOM	3490	CA	ASP B	124	56.471	95.911	-10.806	1.00	63.86
	MOTA	3491	CB	ASP B	124	57.425	96.863	-10.081	1.00	.64.99
	ATOM	3492	CG	ASP B	124	. 58.593	96.115	-9.460	1.00	66.12
15	ATOM	3493	OD1	ASP B	124	58.352	95.082	-8.791	1.00	65.87
	MOTA	3494	OD2	ASP B	124	59.749	96.554	-9.653	1.00	67.14
	ATOM	3495	С	ASP B	124	55.301	95.508	-9.911	1.00	62.01
	MOTA	3496	0	ASP B	124	55.232	95.869	-8.729	1.00	61.22
	MOTA	3497	N	GLU B	125	54.374	94.764	-10.511	1.00	59.15
20	MOTA	3498	CA	GLU B	125	53.175	94.297	-9.842	1.00	55.30
	ATOM	3499	CB	GLU E	125	52.028	95.276	-10.122	1.00	56.22
	ATOM	3500	CG	GLU E	125	52.053	95.871	-11.528	1.00	56.42
	MOTA	3501	CD	GLU E	3 125	50.810	96.673	-11.870	1.00	57.43
	ATOM	3502	OE1	GLU E	3 125	50.176	96.375	-12.911	1.00	56.96
25	MOTA	3503	OE2	GLU F	3 125	50.474	97.601	-11.103	1.00	56.77
	MOTA	3504	C	GLU F	3 125	52.785	92.906	-10.337		53.36
	MOTA	3505	0	GLU I	3 125	53.303	92.413	-11.350	1.00	52.90
	MOTA	3506	N	VAL I	3 126	51.855	92.288	-9.623	1.00	50.42
	MOTA	3507	CA	VAL 1	3 126	51.358	90.962	-9.969	1.00	46.95
30	ATOM	3508	CB	VAL	в 126	52.242	89.843	-9.371	1.00	47.91
	MOTA	3509	CG:	l VAL	в 126	52.128	89.797	-7.851	1.00	48.65
	ATOM	3510	CG:	2 VAL	В 126	51.889	88.500	-9.989	_	47.79
	MOTA	3511	С	VAL	в .126	49.911	90.802	-9.514		43.29
	MOTA	3512	0	VAL	B 126	49.384	91.659	-8.814		43.62
35	ATOM	3513	N	TYR	B 127	49.271	89.716	-9.921	1.00	40.00

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	ATOM	3514	CA	TYR	В	127	47.887	89.479	-9.545	1.00	37.12
	MOTA	3515	CB	TYR	В	127	46.986	89.395	-10.783	1.00	39.32
	ATOM	3516	CG	TYR	В	127	46.672	90.728	-11.434	1.00	42.49
	MOTA	3517	CD1	TYR	В	127	47.438	91.197	-12.501	1.00	42.64
5	ATOM	3518	CE1	TYR	В	127	47.160	92.407	-13.109	1.00	42.93
•	ATOM	3519	CD2	TYR	В	127	45.612	91.513	-10.994	1.00	41.97
	ATOM	3520	CE2	TYR	В	127	45.327	92.728	-11.597	1.00	43.42
	ATOM	3521	CZ	TYR	В	127	46.105	93.170	-12.656	1.00	43.75
	ATOM	3522	ОН	TYR	В	127	45.822	94.377	-13.264	1.00	44.38
10	MOTA	3523	С	TYR	В	127	47.727	88.203	-8.722	1.00	35.28
	ATOM	3524	0	TYR	В	127	48.171	87.126	-9.133	1.00	34.31
	ATOM	3525	N	LEU	В	128	47.045	88.327	-7.584	1.00	30.55
	ATOM	3526	CA .	LEU	В	128	46.768	87.181	-6.727	1.00	26.58
	ATOM	3527	CB	LEU	В	128	46.858	87.554	-5.236	1.00	24.20
15	ATOM	3528	CG	LEU	В	128	46.128	86.602	-4.280	1.00	22.15
	ATOM	3529	CD1	LEU	В	128	46.759	85.218	-4.328	1.00	17.31
	ATOM	3530	CD2	LEU	В	128	46.107	87.156	-2.854	1.00	22.87
	ATOM	3531	С	LEU	В	128	45.376	86.677	-7.040	1.00	22.48
	ATOM	3532	0	LEU	В	128	44.424	87.447	-7.019	1.00	24.60
20	ATOM	3533	N	ASN	В	129	45.252	85.400	-7.333	1.00	21.14
	ATOM	3534	CA	ASN	В	129	43.949	84.834	-7.650	1.00	20.80
	ATOM	3535	СВ	ASN	В	129	43.957	84.125	-9.013	1.00	21.81
	MOTA	3536	CG	ASN	В	129	44.312	85.073	-10.152	1.00	21.32
•	ATOM.	3537	OD1	ASN	В	129	45.468	85.447	-10.318	1.00	22.73
25	ATOM	3538	ND2	ASN	В	129	43.312.	85.479	-10.919	1.00	21.75
	ATOM	3539	С	ASN	В	129	43.472	83.893	-6.556	1.00	20.70
	ATOM	3540	0	ASN	В	129	44.151	82,936	-6.207	1.00	21.20
	MOTA	3541	N	LEU	В	130	42.302	84.183	-6.026	1.00	20.89
	MOTA	3542	CA	LEU	В	130	41.717	83.384	-4.974	1.00	21.65
30	ATOM	3543	CB	LEU	В	130	41.290	84.270	-3.787	1.00	22.41
	ATOM	3544	CG	LEU	В	130	42.398	85.111	-3.150	1.00	22.43
	MOTA	3545	CD1	LEU	В	130	41.814	86.206	-2.267	1.00	23.86
	ATOM	3546	CD2	LEU	В	130	43.361	84.236	-2.370	1.00	22.19
	ATOM	3547	C	LEU	В	130	40.533	82.634	-5.511	1.00	19.68
35	ATOM	3548	Ο.	LEU	В	130	39.582	83.240	-5.980	1.00	21.26

	ATOM	3549	N	VAL B	131	40.600	81.314	-5.442	1.00	18.58
	MOTA	3550	CA	VAL B	131 .	39.521	80.467	-5.926	1.00	20.51
	MOTA	3551	CB	VAL B	131	40.056	79.204	-6.629	1.00	16.75
	MOTA	3552	CG1	VAL B	131	38.945	78.497	-7.366	1.00	14.65
5	ATOM	·3553	CG2	VAL B	131	41.199	79.561	-7.558	1.00	20.04
	MOTA	3554	С	VAL B	131	38.620	80.082	-4.768	1.00	20.58
	ATOM	3555	0	VAL B	131	38.929	79.179	-3.997	1.00	21.73
	ATOM	3556	N	LEU B	132	37.536	80.827	-4.644	1.00	24.39
	ATOM	3557	CA	LEU B	132	36.567	80.675	-3.572	1.00	25.11
10	ATOM	3558	CB	LEU B	132	36.152	82.066	-3.090	1.00	21.67
	ATOM	3559	CG	LEU B	132	37.304	83.031	-2.830	1.00	24.26
	MOTA	3560	CD1	LEU B	132	36.902	84.472	-3.122	1.00	21.82
	ATOM	3561	CD2	LEU B	132	37.809	82.870	-1.403	1.00	22.44
	MOTA	3562	С	LEU B	132	35.329	79.922	-3.985	1.00	27.80
15	MOTA	3563	0	LEU B	132	34.982	79.844	-5.172	1.00	29.52
	MOTA	3564	N	ASP B	133	34.641	79.419	-2.972	1.00	27.43
	MOTA	3565	CA	ASP B	133	33.388	78.709	-3.126	1.00	28.52
	MOTA	3566	CB	ASP B	133	32.825	78.410	-1.728	1.00	30.97
٠	MOTA	3567	CG	ASP B	133	33.214	77.071	-1.149	1.00	33.42
20	MOTA	3568	OD1	ASP B	133	33.227	76.961	0.097	1.00	33.58
	MOTA	3569	OD2	ASP B	133	33.478	76.128	-1.931	1.00	35.77
	ATOM	3570	С	ASP B	133	32.391	79.647	-3.766	1.00	28.01
	MOTA	3571	0	ASP B	133	32.288	80.810	-3.362	1.00	27.90
	MOTA	3572	N	TYR B	134	31.632	79.151	-4.724	1.00	27.47
25	MOTA	3573	CA	TYR B	134	30.627	79.985	-5.354	1.00	26.54
	MOTA	3574	CB	TYR B	134	30.549	79.772	-6.873	1.00	27.48
	ATOM	3575	CG	TYR B	134	29.531	80.682	-7.523	1.00	25.44
	MOTA	3576	CD1	TYR B	134	29.861	81.981	-7.866	1.00	25.68
	ATOM	3577	CE1	TYR E	134	28.932	.82.831	-8.423	1.00	28.12
30	ATOM	3578	CD2	TYR E	134 .	28.232	80.251	-7.756	1.00	27.07
	ATOM	3579	CE2	TYR E	3 134	27.296	81.095	-8.320	1.00	28.14
	MOTA	3580	CZ	TYR E	3 134	27.654	82.384	-8.649	1.00	27.66
	ATOM	3581	OH	TYR F	3 134	26.725	83.235	-9.198	1.00	32.43
	ATOM	3582	С	TYR F	3 134	29.261	79.773	-4.722	1.00	26.49
35	MOTA	3583	0	TYR F	3 134	28.804	78.645	-4.546	1.00	29.00

	MOTA	3584	N	VAL	В	135	28.610	80.873	-4.410	1.00 26	5.03
	MOTA	3585	CA	VAL	В	135	27.281	80.857	-3.832	1.00 27	.01
	MOTA	3586	CB	VAL	В	135	27.302	81.038	-2.296	1.00 27	7.39
	MOTA	3587	CG1	VAL	В	135	25.928	80.771 .	-1.710	1.00 25	5.29
5	MOTA	3588	CG2	VAL	В	135	28.322	80.090	-1.680	1.00 26	5.48
	ATOM	3589	С	VAL	В	135	26.464	81.936	-4.532	1.00 28	3.41
	MOTA	3590	0	VAL	В	135	26.934	83.059	-4.695	1.00 30	0.10
	ATOM	3591	N '	PRO	В	136 ·	25.267	81.581	-5.028	1.00 29	9.44
	ATOM	3592	CD	PRO	В	136	24.680	80.227	-4.933	1.00 29	9.98
10	ATOM	3593	CA	PRO	В	136	24.411	82.496	-5.806	1.00 29	9.90
	MOTA	3594	CB	PRO	В	136	23.382	81.546	-6.434	1.00 30	.14
	ATOM ·	3595	CG	PRO	В	136	23.287	80.419	-5.460	1.00 30	0.40
	MOTA	3596	С	PRO	В	136	23.696	83.605	-5.021	1.00 29	9.47
	MOTA	3597	0	PRO	В	136	23.857	84.783	-5.324	1.00 29	9.46
15	MOTA	3598	N	GLU	В	137	22.860	83.229	-4.068	1.00 28	3.02
	MOTA	3599	CA	GLU	В	137	22.082	84.209	-3.315	1.00 29	9.48
	ATOM	3600	СВ	GLU	В	137	20.783	83.560	-2.816	1.00 33	1.02
	ATOM	3601	CG	GLU	В	137	19.533	83.933	-3.601	1.00 34	1.32
	MOTA	3602	CD	GLU	В	137	19.526	85.381	-4.047	1.00 37	7.83
20	ATOM	3603	OE1	GLU	В	137	19.693	85.627	-5.260	1.00 39	9.93
	MOTA	3604	OE2	GLU	В	137 .	19.358	86.269	-3.185	1.00 39	9.76
	MOTA	3605	С	GLU	В	137	22.846	84.828	-2.138	1.00 27	7.83
	MOTA	3606	0	GLU	В	137	23.893	84.340.	-1.733	1.00 28	3.10
	ATOM	3607	N	THR	В	138	22.266	85.890	-1.581	1.00 2	7.83 ·
25	MOTA	3608	CA	THR	В	138	22.806	86.602	-0.406	1.00 25	5.21
	MOTA	3609	CB	THR	В	138	23.650	87.814	-0.781	1.00 22	2.17
	ATOM	3610	OG1	THR	В	138	22.851	88.827	-1.358	1.00 22	2.19
	ATOM	3611	CG2	THR	В	138	24.827	87.524	-1.675	1.00 2	4.71
	ATOM	3612	С	THR	В	138	21.648	87.088	0.455	1.00 2	3.46
30	ATOM	3613	0	THR	В	138	20.558	87.353	-0.061	1.00 2	2.29
	MOTA	3614	N	VAL	В	139	21.887	87.220	1.767	1.00 2	3.34
	ATOM	3615 _[CA	VAL	В	139	20.840	87.689	2.678	1.00 1	8.25
	ATOM	3616	CB	VAL	В	139	21.342	87.819	4.138	1.00 1	9.10
	ATOM	3617	CG1	VAL	В	139	20.241	88.386	5.030	1.00 1	7.18
35	MOTA	3618	CG2	VAL	В	139	21.787	86.469	4.651	1.00 1	6.04

	ATOM	3619	C	VAL B		139	20.263	89.013	2.201	1.00	16.00
	MOTA	3620	0	VAL B	,	139	19.056	89.222	2.268	1.00	19.23
	MOTA	3621	N	TYR B	3	140	21.131	89.892	1.696	1.00	17.31
	MOTA	3622	CA	TYR B	}	140	20.701	91.194 .	1.182	1.00	18.53
5	MOTA	3623	CB	TYR E	3	140	21.873	91.978	0.586	1.00	17.88
	ATOM	3624	CG	TYR E	3	140	21.438	93.261	-0.094	1.00	22.14
	ATOM	3625	CD1	TYR E	3	140	21.414	94.456	0.599	1.00	22.08
	ATOM	3626	CE1	TYR E	3	140	20.985	95.627	0.010	1.00	24.00
	ATOM	3627	CD2	TYR E	3	140	21.013	93.270	-1.424	1.00	25.34
10	ATOM	3628	CE2	TYR E	3	140	.20.585	94.439	-2.031	1.00	25.37
	ATOM	3629	CZ	TYR E	3	140	20.572	95.618	-1.306	1.00	28.17
-	MOTA	3630	OH	TYR E	3	140	20.144	96.794	-1.898	1.00	29.68
	MOTA	3631	С	TYR F	3	140	19.593	91.054	0.127	1.00	22.25
	MOTA	3632	0	TYR I	3	140	18.589	91.764	0.177	1.00	23.33
15	MOTA	3633	N	ARG I	3	141	19.781	90.155	-0.844	1.00	25.14
	MOTA	3634	CA	ARG I	3	141	18.782	89.976	-1.897	1.00	25.99
	MOTA	3635	CB	ARG I	3	141	19.354	89.162	-3.062	1.00	29.20
	ATOM	3636	CG	ARG I	В	141	20.159	90.003	-4.045	1.00	34.68
	MOTA	3637	CD	ARG 1	В	141	21.396	89.263	-4.550	1.00	39.35
20	ATOM	3638	NE	ARG 1	В	141	21.049	88.183	-5.473		45.84
	MOTA	3639	CZ	ARG :	В	141	20.518	88.374	-6.691		48.75
	MOTA	3640	NH1	ARG	В	141	20.306	89.608	-7.159		50.02
	MOTA	3641	NH2	ARG	В	141	20.204	87.324	-7.448		49.98
	MOTA	3642	С	ARG	В	141	17.532	89.321	-1.341		25.44
25	ATOM	3643	0	ARG	В	141	16.410	89.751	-1.626	•	25.68
	MOTA	3644	N	VAL	В	142	17.716	88.287	-0.532		25.77
	MOTA	3645	CA	VAL	В	142	16.573	87.613	0.057		25.48
	ATOM	3646	CB	VAL	В	142	16.994	86.424	0.945		26.10
	MOTA	3647	CG1	VAL	В	142	15.814	85.905	1.747		25.96
30	MOTA	3648	CG2	. VAL	В	142	17.586	85.313	0.088		27.08
	MOTA	3649	С	VAL	В	142	15.734	88.610	0.850		25.06
	MOTA	3650	0	VAL	В	142	14.512	88.600	0.763		27.10
	MOTA	3651	N	ALA	B	3 143	16.409		1.598		25.37
	MOTA	3652	CA	ALA	B	3 143	15.738		2.397		25.38
35	ATOM	3653	CB	ALA	E	3 143	16.744	91.238	3.283	1.00	23.30

	ATOM	3654	С	ALA	В	143	15.005	91.522	1.507	1.00	25.25
	MOTA	3655	0	ALA	В	143	13.821	91.794	1.712	1.00	25.01
	ATOM	3656	N	ARG	В	144	15.714	92.060	0.508	1.00	27.14
	ATOM	3657	CA	ARG	В	144	15.125	93.023	-0.427	1.00	27.56
5	ATOM	3658	СВ	ARG	В	144	16.141	93.423	-1.499	1.00	28.99
•	ATOM	3659	CG	ARG	В	144	15.608	94.477	-2.466	1.00	31.54
	MOTA	3660	CD	ARG	В	144	16.704	95.035	-3.353	1.00	32.11
	ATOM	3661	NE	ARG	В	144	17.293	94.000	-4.198	1.00	35.33
	MOTA	3662	CZ	ARG	В	144	18.226	94.223	-5.123	1.00	35.49
10	MOTA	3663	NHI	ARG	В	144	18.678	95.457	-5.357	1.00	35.51
	ATOM	3664	NH2	ARG	В	144	18.709	93.199	-5.818	1.00	36.90
	MOTA	3665	C	ARG	В	144	13.872	92.448	-1.089	1.00	27.74
	MOTA	3666	0	ARG	В	144	12.865	93.147	-1.255	1.00	30.06
	MOTA	3667	Ņ	HIS	В	145	13.930	91.171	-1.440	1.00	27.38
15	ATOM	3668	CA	HIS	В	145	12.800	90.494	-2.057	1.00	29.82
	ATOM	3669	CB	HIS	В	145	13.153	89.033	-2.358	1.00	33.31
	ATOM	3670	CG	HIS	В	145	12.098	88.302	-3.123	1.00	38.70
	MOTA	3671	CD2	HIS	В	145	11.584	87.058	-2.960	1.00	41.14
	ATOM	3672	ND1	HIS	В	145	11.429	88.852	-4.202	1.00	41.54
20	MOTA	3673	CE1	HIS	В	145	10.549	87.978	-4.665	1.00	42.00
	MOTA	3674	NE2	HIS	В	145	10.623	86.880	-3.929	1.00	41.98
	MOTA	3675	С	HIS	В	145	11.558	90.575	-1.167	1.00	29.00
	ATOM	3676	0	HIS	В	145	10.507	91.053	-1.598	1.00	30.08
	ATOM	3677	N	TYR	В	146	11.683	90.120	0.081	1.00	28.13
25	MOTA	3678	CA	TYR	В	146	10.565	90.167	1.016	1.00	25.81
	MOTA	3679	ĊB	TYR	В	146	10.919	89.471	2.332	1.00	23.53
	MOTA	3680	CG	TYR	В	146	10.782	87.978	2.242	1.00	19.02
	ATOM	3681	CD1	TYR	В	146	11.846	87.193	1.826	1.00	18.11
	MOTA	3682	CE1	TYR	В	146	11.719	85.829	1.702	1.00	17.01
30	ATOM	3683	CD2	TYR	В	146	9.581	87.357	2.536	1.00	19.30
	ATOM	3684	CE2	TYR	В	146	9.446	85.991	2.421	1.00	18.95
	. ATOM	3685	CZ	TYR	В	146	10.520	85.233	2.001	1.00	18.86
	ATOM	3686	OH	TYR	В	146	10.388	83.873	1.879	1.00	23.47
	MOTA	3687	С	TYR	В	146	10.133	91.603	1.271	1.00	26.52
35	MOTA	3688	0	TYR	В	146	8.943	91.910	1.271	1.00	27.02

	MOTA	3689	N	SER I	В	147	11.114	92.476	1.480	1.00	29.00
	ATOM	3690	CA	SER I	В	147	10.864	93.890	1.737	1.00	31.27
	MOTA	3691	CB	SER :	В	147	12.189	94.631	1.913	1.00	32.96
	ATOM	3692	OG	SER :	В	147	12.065	95.669	2.870	1.00	37.24
5	MOTA	3693	С	SER	В	147	10.040	94.540	0.622	1.00	33.59
	ATOM	3694	0	SER	В	147	9.102	95.290	0.894	1.00	34.13
	ATOM	3695	N	ARG	В	148	10.392	94.254	-0.635	1.00	34.97
	MOTA	3696	CA	ARG	В	148	9.671	94.825	-1.774	1.00	35.55
	MOTA	3697	CB	ARG	В	148	10.387	94.494	-3.085	1.00	36.04
10	MOTA	3698	.CG	ARG	В	148	11.721	95.209	-3.245	1.00	36.48
	MOTA	3699	CD	ARG	В	148	12.555	94.593	-4.360	1.00	37.75
	ATOM	3700	NE	ARG	В	148	13.591	95.508	-4.847	1.00	40.00
	MOTA	3701	CZ	ARG	В	148	14.421	95.236	-5.860	1.00	40.69
	ATOM	3702	NH1	ARG	В	148	14.359	94.070	-6.494	1.00	40.58
15.	MOTA	3703	NH2	ARG	В	148	15.321	96.137	-6.237	1.00	41.76
	ATOM	3704	С	ARG	В	148	8.228	94.325	-1.816	1.00	35.37
	MOTA	3705	0	ARG	B	148	7.309	95.082	-2.131	1.00	36.98
	ATOM	3706	N	ALA	В	149	8.032	93.053	-1.484	1.00	34.57
	MOTA	3707	CA	ALA	В	149	6.697	92.460	-1.476	1.00	33.48
20	MOTA	3708	CB	ALA	В	149	6.780	90.956	-1.675	1.00	33.34
	MOTA	3709	С	ALA	В	149	5.918	92.790	-0.203	1.00	33.34
	MOTA	3710.	0	ALA	В	149	4.840	92.253	0.004	1.00	32.82
	ATOM	3711	N	LYS	В	150	6.469	93.676	0.644	1.00	35.63
	MOTA	3712	CA	LYS	В	150	5.824	94.076	1.899	1.00	35.93
25	ATOM	3713	CB	LYS	В	150	4.575	94.916	1.624	1.00	36.80
	MOTA	3714	CG	LYS	В	150	4.887	96.330	1.157	1.00	37.59
	MOTA	3715	CD	LYS	В	150	5.543	97.162	2.254	1.00	38.68
	MOTA.	3716	CE	LYS	В	150	6.378	98.302	1.674	1.00	39.17
	MOTA	3717	NZ	LYS	В	150	5.826	99.646	2.024	1.00	40.69
30	MOTA	3718	С	LYS	В	150	5.486	92.851	2.745	1.00	35.84
	MOTA	3719	0	LYS	В	150	4.357	92.658	3.192	1.00	35.50
	MOTA	3720	N	GLN	В	151	6.495	92.026	2.938	1.00	36.24
	ATOM	3721	CA	GLN	В	151	6.387	90.802	3.701	1.00	35.89
	MOTA	3722	CB	GLN	В	151	6.400	89.605	2.749	1.00	37.28
35	MOTA	3723	CG	GLN	В	151	5.187	88.703	2.839	1.00	38.89

	MOTA	3724	CD	GLN	В	151	4.668	88.316	1.467	1.00	41.33
	ATOM	3725	OE1	GLN	В	151	5.446	88.066	0.541	1.00	41.35
	ATOM	3726	NE2	GLN	В	151	3.347	88.268	1.330	1.00	42.23
	MOTA	3727	С	GLN	В	151	7.583	90.687	4.612	1.00	35.52
5	MOTA	3728	0	GLN	B	151	8.669	91.166	4.285	1.00	35.18
	MOTA	3729	N	THR	В	152	7.394	90.033	5.741	1.00	35.74
	ATOM	3730	CA	THR	В	152	8.482	89.843	6.677	1.00	35.93
	MOTA	3731	CB	THR	В	152	7.980	89.947	8.131	1.00	36.72
	ATOM	3732	OG1	THR	B	152	8.812	89.221	9.025	1.00	40.21
10	MOTA	3733	CG2	THR	В	152	6.551	89.487	8.337	1.00	36.78
	MOTA	3734	С	THR	В	152	9.145	88.500	6.416	1.00	32.95
	ATOM	3735	0	THR	В	152	8.466	87.501	6.200	1.00	33.95
	ATOM	3736	N	LEU	В	153	10.464	88.474	6.438	1.00	31.92
•	ATOM	3737	CA	LEU	В	153	11.184	87.232	6.217	1.00	30.87
15	MOTA	3738	CB	LEU	В	153	12.686	87.508	6.165	1.00	31.70
	MOTA	3739	CG	LEU	В	153	13.605	86.301	5.982	1.00	32.12
	ATOM	3740	CD1	LEU	В	153	13.379	85.648	4.627	1.00	32.63
	MOTA	3741	CD2	LEU	В	153	15.055	86.721	6.139	1.00	33.53
	MOTA	3742	С	LEU	В	153	10.860	86.277	7.356	1.00	30.19
20	MOTA	3743	0	LEU	В	153	11.119	86.594	8.510	1.00	31.69
	MOTA	3744	N	PRO	В	154	10.266	85.102	7.055	1.00	29.41
	MOTA	3745	CD	PRO	В	154	9.898	84.640 ·	5.696	1.00	27.70
	ATOM'	3746	CA	PRO	В	154	9.891	84.124	8.080	1.00	27.35
	ATOM	3747	CB	PRO	В	154	9.714	82.836	7.280	1.00	28.38
25	MOTA	3748	CG	PRO	В	154	9.215	83.315	5.949	1.00	28.03
	ATOM	3749	С	PRO	В	154	10.962	83.978	9.159	1.00	25.58
	ATOM	3750	0	PRO	В	154	12.153	83.809	8.863	1.00	25.12
	ATOM	3751	N	VAL	В	155	10.527	84.082	10.418	1.00	24.34
	ATOM	3752	CA	VAL	В	155	11.435	83.997	11.567	1.00	22.14
30	MOTA	3753	CB	VAL	В	155	10.689	84.144	12.923	1.00	23.51
	ATOM	3754	CG1	VAL	В	155	11.560	83.672	14.082	1.00	22.33
	ATOM	3755	CG2	. VAL	В	155	10.293	85.598	13.127	1.00	20.79
	MOTA	3756	С	VAL	В	155	12.346	82.768	11.539	1.00	19.24
	ATOM	3757	0	VAL	В	155	13.489	82.840	12.005	1.00	21.30
35	ATOM	3758	N	ILE	В	156	11.872	81.644	10.981	1.00	19.80

	MOTA	3759	CA	ILE :	В	156	12.718	80.441	10.908	1.00	20.19
	MOTA	3760	CB	ILE :	B.	156	11.980	79.211	10.311	1.00	23.70
	MOTA	3761	CG2	ILE :	В	156	11.512	79.480	8.882	1.00	20.74
	MOTA	3762	CG1	ILE :	B	156	12.872	77.963	10.344	1.00	23.22
5	ATOM	3763 *	CD1	ile :	B	156	13.199	77.470	11.740	1.00	27.05
	ATOM	3764	С	ILE	В	156	14.012	80.713	10.125	1.00	20.85
	MOTA	3765	0	ILE	В	156	15.064	80.187	10.460	1.00	23.05
	MOTA	3766	N	TYR	В	157	13.931	81.546	9.088	1.00	21.98
	MOTA	3767	CA	TYR	B	157	15.103	81.881	8.267	1.00	21.22
10	ATOM	3768	CB	TYR	В	157	14.660	82.525	6.944	1.00	23.30
	ATOM	3769	CG	TYR	B	157	13.948	81.576	6.027	1.00	23.20
	ATOM	3770	CD1	TYR	В	157	12.631	81.796	5.662	1.00	26.34
	ATOM	3771	CE1	TYR	В	157	11.970	80.918	4.830	1.00	26.40
	ATOM	3772	CD2	TYR	B	157	14.592	80.450	5.531	1.00	24.66
15	ATOM	3773	CE2	TYR	В	157	13.941	79.568	4.694	1.00	25.59
	MOTA	3774	CZ	TYR	В	157	12.634	79.806	4.350	1.00	27.07
	ATOM	3775	OH	TYR	В	157	11.976	78.922	3.532	1.00	32.84
	MOTA	3776	С	TYR	В	157	16.057	82.819	8.990	1.00	20.56
	ATOM	3777	0	TYR	В	157	17.281	82.735	8.817	1.00	19.78
20	ATOM	3778	N	VAL	В	158	15.496	83.717	9.808	1.00	20.27
	MOTA	3779	CA	VAL	В	158	16.314	84.649	10.563	1.00	20.35
	ATOM	3780	CB	VAL	В	158	15.452	85.694	11.311	1.00	21.37
	ATOM	3781	CG1	VAL	В	158	16.338	.86.766	11.943	1.00	19.60
	ATOM	∵3782	CG2	VAL	В	158	14.457	86.336	10.351	1.00	18.28
25	ATOM	3783	С	VAL	В	158	17.180	83.862	11.537	1.00	18.97
	MOTA	3784	0	VAL	В	158	18.387	84.016	11.565	1.00	23.65
	MOTA	3785	N	LYS	В	159	16.551	82:979	12.299	1.00	20.72
	MOTA	3786	CA	LYS	В	159	17.272	82.126	13.254	1.00	19.58
	MOTA	3787	CB	LYS	В	159	16.303	81.133	13.901	1.00	17.16
30	ATOM	3788	CG	LYS	В	159	15.249	81.785	14.788	1.00	20.51
	ATOM	3789	CD	LYS	В	159	14.393	80.735	15.487	1.00	19.90
	ATOM	3790	CE	LYS	В	159	13.268	81.368	16.279	1.00	21.69
	ATOM	3791	NZ	LYS	В	159	12.223	80.372	16.638	1.00	22.17
•	ATOM	3792	С	LYS	В	159	18.405	81.368	12.570	1.00	18.48
35	ATOM	3793	0	LYS	В	159	19.553	81.433	13.006	1.00	17.43

	MOTA	3794	N	LEU 1	В	160	18.065	80.643	11.482	1.00	19.66
	ATOM	3795	CA	LEU !	В.	160	19.048	79.860	10.719	1.00	18.83
	ATOM	3796	СВ	LEU I	В	160	18.379	79.163	9.522	1.00	19.66
	ATOM	3797	CG	LEU :	В	160	17.774	77.795	9.788	1.00	19.93
5	ATOM	3798	CD1	LEU	В	160	16.700	77.486	8.765	1.00	21.83
	ATOM	3799	CD2	LEU	В	160	18.854	76.724	9.801	1.00	21.52
	ATOM	3800	С	LEU	В	160	20.186	80.721	10.216	1.00	16.03
	MOTA	3801	0	LEU	В	160	21.345	80.349	10.341	1.00	16.78
	ATOM	3802	N	ŤYR	В	161 .	19.857	81.869	9.627	1.00	17.43
10	MOTA	3803	CA	TYR	В	161	20.888	82.762	9.089	1.00	19.10
	MOTA	3804	СВ	TYR	В	161	20.250	83.920	8.284	1.00	19.88
	ATOM .	3805	CG	TYR	B	161	19.476	83.557	7.024	1.00	24.99
	MOTA	3806	CD1	TYR	В	161	19.463	82.271	6.496	1.00	25.12
	MOTA	3807	CE1	TYR	В	161	18.725	81.975	5.358	1.00	29.18
15	MOTA	3808	CD2	TYR	В	161	18.735	84.530	6.373	1.00	26.00
	ATOM	3809	CE2	TYR	В	161	18.004	84.249	5.241	1.00	29.30
	MOTA	3810	CZ	TYR	В	161	17.998	82.976	4:737	1.00	30.29
	MOTA	3811	ОН	TYR	В	161	17.254	82.700	3.612	1.00	33.10
	MOTA	3812	С	TYR	В	161	21.740	83.366	10.221	1.00	18.94
20	MOTA	3813	0	TYR	В	161	22.974	83.354	10.182	1.00	17.38
	MOTA	3814	N	MET	В	162	21.061	83.926	11.221	1.00	18.27
	ATOM	3815	CA	MET	В	162	21.767	84.560	12.347	1.00	18.73
	ATOM .	3816	СВ	MET	В	162	20.770	85.237	13.288	1.00	16.64
	ATOM	3817	CG	MET	В	162	20.235	86.526	12.724	1.00	16.75
25	ATOM	3818	SD	MET	В	162	21.522	87.547	11.984	1.00	21.72
	MOTA	3819	CE	MET	В	162	22.654	87.807	13.364	1.00	22.96
	MOTA	3820	С	MET	В	162	22.656	83.584	13.078	1.00	13.97
	MOTA	3821	0	MET	В	162	23.784	83.906	13.407	1.00	18.33
	MOTA	3822	N	TYR	В	163	22.146	82.382	13.301	1.00	16.83
30	ATOM	3823	CA	TYR	В	163	22.891	81.317	13.994	1.00	17.57
•	MOTA	3824	СВ	TYR	В	163	21.998	80.075	14.143	1.00	16.83
	MOTA	3825	CG	TYR	E	163	22.689	78.913	14.842	1.00	18.42
	MOTA	3826	CD:	L TYR	E	163	22.814	78.874	16.240	1.00	16.94
	ATOM	3827	CE:	l TYR	E	163	23.444	77.815	16.873	1.00	17.73
35	ATOM	3828	CD	2 TYR	E	3 163	23.214	77.862	14.106	1.00	16.91

	MOTA	3829	CE2	TYR	В	163	23.842	76.804	14.718	1.00	19.62
	ATOM	3830	CZ	TYR	В	163	23.957	76.780	16.109	1.00	22.45
	ATOM	3831	ОН	TYR	В	163	24.585	75.723	16.715	1.00	19.94
	ATOM	3832	С	TYR	В	163	24.183	80.938	13.281	1.00	18.55
5	ATOM	3833	0	TYR	В	163	25.267	80.837	13.907	1.00	18.64
	ATOM	3834	N	GLN	В	164	24.077	80.716	11.958	1.00	17.45
	ATOM	3835	CA	GLN	В	164	25.239	80.342	11.166	1.00	13.31
	ATOM	3836	CB	GLN	В	164	24.817	79.910	9.762	1.00	15.13
	ATOM	3837	CG	GLN	В	164	24.007	78.628	9.747	1.00	16.53
10	ATOM	3838	CD	GLN	В	164	23.455	78.316	8.367	1.00	16.29
	MOTA	3839	OE1	GLN	В	164	24.142	77.720	7.550	1.00	16.87
:	ATOM	3840	NE2	GLN	В	164	22.224	78.727	8.104	1.00	13.57
	ATOM	3841	C	GLN	В	164	26.239	81.472	11.131	1.00	9.92
	MOTA	3842	0	GLN	В	164	27.430	81.241	11.174	1.00	12.36
15	ATOM	3843	N	LEU	В	165	25.733	82.703	11.107	1.00	11.26
	MOTA	3844	CA	LEU	В	165	26.581	83.890	11.129	1.00	13:08
	MOTA	3845	CB	LEU	В	165	25.702	85.138	10.991	1.00	12.81
	ATOM	3846	CG	LEU	В	165	26.346	86.410	10.423	1.00	15.34
	ATOM	3847	CDI	LEU	В	165	25.759	87.659	11.062	1.00	12.66
20	ATOM	3848	CD2	LEU	В	165	27.854	86.395	10.525	1.00	18.57
	ATOM	3849	С	LEU	В	165	27.366	83.950	12.456	1.00	12.95
	MOTA	3850	0	LEU	В	165	28.573	84.144	12.467	1.00	16.32
	MOTA	3851	N	PHE	В	166	26.676	83.768	13.585	1.00	14.47
	ATOM	3852	CA	PHE	В	166	27.375	83.790	14.876	1.00	12.97
25	MOTA	3853	CB	PHE	В	166	26.386	83.728	16.043	1.00	11.30
•	MOTA	3854	CG	PHE	В	166	25.697	85.037	16.242	1.00	6.37
	ATOM	3855	CD1	PHE	В	166	24.333	85.121	16.220	1.00	6.85
	ATOM	3856	CD2	PHE	В	166	26.429	86.183	16.440	1.00	7.66
	ATOM	3857	CE1	PHE	В	166	23.695	86.326	16.391	1.00	5.07
30	MOTA	3858	CE2	PHE	В	166	25.800	87.399	16.616	1.00	9.58
	ATOM	3859	CZ	PHE	В	166	24.428	87.466	16.589	1.00	7.06
	ATOM	3860	С	PHE	В	166	28.418	82.689	14.920	1.00	10.95
	ATOM	3861	0	PHE	B	166	29.570	82.930	15.309	1.00	16.03
	MOTA	3862	N	ARG	В	167	28.039	81.497	14.462	1.00	12.53
35	MOTA	3863	CA	ARG	·B	167	28.963	80.364	14.400	1.00	13.60

	MOTA	3864	СВ	ARG B	167		28.275	79.162	13.750	1.00 18.63
	MOTA	3865	CG	ARG B	167	-	27.668	78.171	14.734	1.00 19.55
	MOTA	3866.	CD	ARG B	167		27.437	76.814	14.088	1.00 19.56
	ATOM	3867	NE	ARG B	167		28.676	76.045	13.967	1.00 20.35
5	AŢOM	3868	CZ	ARG B	167		28.785	74.891	13.299	1.00 16.47
	ATOM	3869	NH1	ARG B	167		27.737	74.355	12.692	1.00 20.44
	ATOM	3870	NH2	ARG B	167		29.944	74.274	13.240	1.00 18.83
	MOTA	3871	С	ARG B	167		30.232	80.715	13.613	1.00 17.56
	ATOM	3872	0	ARG B	167		31.372	80.451	14.062	1.00 19.20
10	MOTA	3873	N	SER B	168		30.065	81.324	12.435	1.00 17.30
•	ATOM	3874	CA	SER B	168		31.246	81.695	11.657	1.00 17.33
_	ATOM	3875	СВ	SER E	168		30.870	82.151	10.230	1.00-15.58
·	ATOM	3876	OG	SER E	3 168		30.353	83.476	10.201	1.00 13.88
	ATOM	3877	С	SER	3 168		32.033	82.777	12.402	1.00 15.51
15	ATOM	3878	0	SER E	3 168		33.263	82.845	12.329	1.00 16.25
	MOTA	3879	N	LEU H	3 169		31.316	83.615	13.137	1.00 15.49
	ATOM	3880	CA	LEU I	3 169		31.973	84.675	13.915	1.00 17.05
	MOTA	3881	СВ	LEU 1	B 169		30.954	85.677	14.436	1.00 17.09
	MOTA	3882	CG	LEU 1	в 169		30.401	86.619	13.363	1.00 18.69
20	MOTA	3883	CDI	L LEU	в 169		29.354	87.569	13.922	1.00 13.84
	MOTA	3884	CD2	2 LEU	в 169		31.533	87.377	12.666	1.00 14.52
	ATOM	3885	С	LEU	в 169		32.822	84.082	15.031	1.00 15.99
	MOTA	3886	0	LEU	в 169	•	33.980	84.464	15.214	1.00.16.48
	ATOM	3887	N	ALA	в 170	}	32.250	83.107	15.745	1.00 18.87
25	MOTA	3888	CA	ALA	в 170)	32.943	82.407	16.845	1.00 21.00
	MOTA	3889	CB	ALA	B 170)	32.012	81.352	17.449	1.00 19.79
	ATOM	3890	С	. ALA	в 170)	34.220	81.741	16.352	1.00 21.82
	MOTA	3891	Ö	ALA	в 170)	35.266	81.760	17.026	1.00 22.36
	MOTA	3892	N	TYR	в 171	L	34.127	81.144	15.165	1.00 23.15
30	MOTA	3893	CA	TYR	в 17:	l.	35.256	80.458	14.558	1.00 19.25
	ATOM	3894	CE	3 TYR	в 17	1	34.826	79.705	13.297	1.00 20.50
	MOTA	3895	c c	S TYR	в 17	1	35.971	78.969	12.643	1.00 18.22
	ATOM	3896	5 CI	O1 TYR	в 17	1.	36.368	3 77.727	7 13.110	1.00 15.97
٠	MOTA	3897	7 CI	El TYR	в 17	1	37.410	77.05	12.521	1.00 18.29
35	ATOM	. 3898	3 C1	D2 TYR	в 17	1	36.65	6 79.52	3 11.560	1.00 16.49
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	MOTA	3899	CE2	TYR E	3 ;	17.1	37.705	78.849	10.964	1.00	15.82
	MOTA	3900	CZ	TYR E	3	171	38.073	77.619	11.446	1.00	18.15
	MOTA	3901	OH	TYR E	3	171	39.103	76.939	10.859	1.00	21.31
	MOTA .	3902	С	TYR: E	3	171	36.394	81.393	14.236	1.00	17.82
5	MOTA	3903	0	TYR E	3	171	37.544	81.086	14.528	1.00	22.52
	ATOM.	3904	N	ILE E	3	172	36.093	82.520	13.616	1.00	18.32
	MOTA	3905	CA	ILE E	3	172	37.147	83.471	13.249	1.00	18.09
	MOTA	3906	CB	ILE E	3	172	36.701	84.470	12.158	1.00	16.91
	MOTA	3907	CG2	ILE E	3	172	36.617	83.787	10.793	1.00	18.79
10	ATOM	3908	CG1	ILE E	3	172	35.361	85.101	12.516	1.00	16.59
	ATOM	3909	CD1	ILE E	3	172	35.267	86.556	12.121	1.00	17.41
	ATOM	3910	C	ILE F	3	172	37.676	84.232	14.471	1.00	17.72
	MOTA	3911	0	ILE E	3	172	38.894	84.411	14.624	1.00	16.48
	ATOM	3912	N	HIS H	3	173	36.759	84.664	15.346	1.00	18.14
15	ATOM	3913	CA	HIS H	3	173	37.161	85.380	16.566	1.00	18.28
	ATOM	3914	CB	HIS I	3	173	35.939	85.810	17.381	1.00	14.98
	ATOM ·	3915	CG	HIS I	В	173	35.179	86.918	16.731	1.00	12.61
	ATOM	3916	CD2	HIS I	3	173	35.510	87.730	15.691	1.00	15.00
	ATOM	3917	ND1	HIS I	3	173	33.924	87.306	17.118	1.00	15.31
20	ATOM	3918	CE1	HIS I	В	173	33.508	88.305	16.349	1.00	13.51
	ATOM	3919	NE2	HIS I	В	173	34.457	88.579	15.479	1.00	11.84
	ATOM	3920	C	HIS !	В	173	38.123	84.507	17.380	1.00	18.31
	ATOM	3921	0	HIS	В	173	39.122	84.995	17.886	1.00	23.85
	ATOM	3922	N	SER :	В	174	37.845	83.200	17.436	1.00	21.25
25	MOTA	3923	CA	SER	В	174	38.706	82.222	18.136	1.00	21.23
	ATOM	3924	CB	SER	В	174	38.120	80.800	18.017	1.00	23.92
	MOTA	3925	OG	SER	В	174	38.766	80.026	17.009	1.00	29.48
	ATOM	3926	C	SER	В	174	40.176	82.273	17.675	1.00	22.44
	ATOM	3927	0	SER	В	174	41.083	81.828	18.388	1.00	20.91
30	ATOM	3928	N	PHE	В	175	40.410	82.829	16.482	1.00	22.81
	ATOM	3929	CA	PHE	В	175	41.758	82.953	15.930	1.00	20.67
	MOTA	3930	СВ	PHE	В	175	41.740	82.656	14.418	1.00	23.12
	ATOM	3931	CG	PHE	В	175	41.717	81.196	14.049	1.00	21.93
	MOTA	3932	CD1	PHE	В	175	42.868	80.436	14.112	1.00	21.49
35	MOTA	3933	CD2	PHE	В	175	40.541	80.593	13.633	1.00	22.75

	ATOM	3934	CE1	PHE B	175	42.847	79.097	13.770	1.00 2	4.14
,	MOTA	3935	CE2	PHE B	175	40.512	79.257	13.293	1.00 2	1.54
	ATOM	3936	CZ	PHE B	175	41.666	78.507	13.362	1.00 2	0.39
	MOTA	3937	С	PHE B	175	42.299	84.367	16.144	1.00 2	20.00
5	ATOM	3938	0	PHE B	175	43.457	84.645	15.849	1.00 2	21.75
	ATOM	3939	N	GLY B	176	41.442	85.265	16.624	1.00 1	.8.95
	ATOM	3940	CA	GLY B	176	41.837	86.654	16.833	1.00 2	20.05
	ATOM	3941	С	GLY B	176	41.498	87.512	15.617	1.00	19.66
•	MOTA	3942	0	GLY B	176	41.796	88.705	15.568	1.00	L7.74 .
10	ATOM	3943	N	ILE B	177	40.885	86.877	14.626	1.00	19.43
	ATOM	3944	CA	ILE B	177	40.521	87.540	13.388	1.00	17.66
	ATOM	3945	ÇB	ILE B	177	40.471	86.528	12.218	1.00	18.89
	MOTA	3946	CG2	ILE B	177	39.866	87.169	10.970	1.00	22.27
	MOTA	3947	CG1	ILE E	177	41.864	85.976	11.924	1.00	18.79
15	MOTA	3948	CD1	ILE E	3 177	41.850	84.580	11.333	1.00	18.07
	ATOM	3949	С	ILE E	3 177	39.186	88,252	13.460	1.00	13.18
	ATOM	3950	0	ILE E	3 177	38.154	87.652	13.694	1.00	14.34
	MOTA	3951	N	CYS I	3 178	39.212	89.529	13.163	1.00	14.13
	ATOM	3952	ĊA	CYS I	3 178	38.003	90.313	13.097	1.00	15.75
20	MOTA	3953	CB	CYS I	3 178	38.207	91.633	13.822	1.00	12.82
	ATOM	3954	SG	CYS 1	В 178	36.704	92.568	14.016	1.00	20.44
	ATOM	3955	С	CYS :	в 178	37.693	.90.561	11.592		16.81
	ATOM	3956	0	CYS	в 178	38.616	90.797	10.812	1.00	18.44
	ATOM	3957	N	HIS	В 179	36.420	90.470	11.211		17.46
25	MOTA	3958	CA	HIS	в 179	35.973	90.648	9.823		18.34
	MOTA	3959	CB	HIS	В 179	34.557	90.106	9.660		16.84
	ATOM	3960	CG	HIS	В 179	34.198	89.789			18.96
4	ATOM	3961	. CD	2 HIS	В 179	34.490	88.717			18.32
	MOTA	3962	ND	1 HIS	B 179	33.444				19.17
30	MOTA	3963	3 CE	1 HIS	В 179	33.280				16.74
	ATOM	3964	A NE	2 HIS	B 179	33.904				15.67
	MOTA	3965	5 C	HIS	B 179	36.030	92.120			20.37
	MOTA	396	6 0	HIS	В 179	36.783	•	_		19.08
	MOTA	396	7 N	ARG	B 180	35.258				19.56
35	ATOM	396	8 C	A ARG	В 180	35.198	94.38	9.983	1.00	19.52

	MOTA	3969	СВ	ARG B	180	36.596	94:975	9.873	1.00	21.91
•	ATOM	3970	CG	ARG B	180.	37.585	94.396	10.859	1.00	18.09
	ATOM	3971	CD	ARG B	180	38.672	95.403	11.177	1.00	21.06
	MOTA	3972	NE	ARG B	180	39.531	95.661	10.019	1.00	22.36
5	ATOM	3973	CZ	ARG B	180	40.540	96.527	10.013	1.00	19.95
	ATOM	3974	NH1	ARG B	180	40.716	97.382	11.028	1.00	22.70
	ATOM	3975	NH2	ARG B	180	41.369	96.553	8.981	1.00	18.96
	ATOM	3976	С	ARG B	180	34.323	94.837	8.799	1.00	20.34
	ATOM	3977	0	ARG B	180	34.320	96.016	8.432	1.00	20.98
10	ATOM	3978	N	ASP B	181	33.546	93.923	8.246	1.00	21.43
•	ATOM	3979	CA	ASP B	181	32.651	94.257	7.150	1.00	23.13
•	ATOM	3980	СВ	ASP B	181	33.397	94.205	5.814	1.00	22.99
	ATOM	3981	CG	ASP B	181	32.706	94.987	4.716	1.00	24.00
•	ATOM	3982	OD1	ASP B	181 .	31.738	95.710	5.017	1.00	22.68
15	ATOM	3983	OD2	ASP B	181	33.143	94.873	3.546	1.00	26.09
	MOTA	3984	С	ASP B	181	31.431	93.346	7.126	1.00	24.10
	ATOM	3985	0	ASP B	181	31.030	92.837	6.071	1.00	27.13
•	ATOM	3986	N	ILE B	182	30.831	93.151	8.291	1.00	22.83
	MOTA	3987	CA	ILE B	182	29.655	92.317	8.422	1.00	20.44
20	ATOM	3988	CB	ILE B	182.	29.466	91.833	9.872	1.00	21.37
	ATOM	3989	CG2	ILE B	182	28.127	91.131	10.053	1.00	21.22
	MOTA	3990	CG1	ILE B	182	30.621	90.919	10.273	1.00	19.44
	MOTA	3991	CD1	ILE B	182	30.463	89.488	9.800	1.00	19.22
	ATOM	3992	С	ILE B	182	28.421	93.068	7.972	1.00	20.80
25	ATOM	3993	.0	ILE B	182	28.086	94.108	8.523	1.00	20.95
	ATOM	3994	N	LYS B	183	27.767	92.524	6.941	1.00	19.52
	ATOM	3995	CA	LYS B	183	26.573	93.121	6.356	1.00	16.61
	ATOM	3996	CB	LYS B	183	26.971	94.319	5.515	1.00	15.49
	ATOM	3997	CG	LYS B	183	28.126	94.032	4.573	1.00	15.33
30	ATOM	3998	CD	LYS B	183	28.436	95.248	3.726	1.00	17.88
	MOTA	3999	CE	LYS B	183	29.187	94.884	2.460	1.00	17.85
. •	MOTA	4000	ΝZ	LYS B	183	29.949	96.042	1.927	1.00	19.34
	MOTA	4001	С	LYS B	183	25.826	92.079	5.515	1.00	14.55
	ATOM	4002	0	LYS B	183	26.390	91.051	5.147	1.00	13.32
35 ·	ATOM	4003	N	PRO B	184	24.546	92.306	5.234	1.00	13.82
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	ATOM	4004	CD	PRO B	184	23.783	93.487	5.647	1.00 1	3.63
	MOTA	4005	CA	PRO B	184	23.719.	91.351	4.478	1.00 1	6.50
	MOTA	4006	СВ	PRO B	184	22.386	92.079	4.305	1.00 1	.4.92
	ATOM	4007	CG	PRO B	184	22.357	93.062 .	5.429	1.00 1	5.66
5	ATOM	4008	C	PRO B	184	24.310	90.922	3.112 ·	1.00 1	7.86
	ATOM	4009	0	PRO B	184	24.079	89.804	2.674	1.00 2	21.42
	ATOM.	4010	N	GLN B	185	25.066	91.791	2.449	1.00	18.44
	MOTA	4011	CA	GLN B	185	25.639	91.416	1.158	1.00 2	21.79
	MOTA	4012	CB	GLN B	185	26.030	92.638	0.309	1.00 2	24.61
10	ATOM	4013	CG	GLN B	·185	26.490	93.856	1.102	1.00	32.20
	ATOM	4014	CD	GLN B	185	25.342	94.744	1.579	1.00	32.15
	ATOM	4015	OE1	GLN B	185	24.883	95.637	0.862	1.00	33.73
	MOTA	4016	NE2	GLN B	185	24.881	94.505	2.795	1.00	28.11
	MOTA	4017	С	GLN B	185	26.802	90.437	1.306	1.00	21.53
15	ATOM	4018	0	GLN B	185	27.117	89.683	0.379	1.00	16.27
	ATOM	4019	N	ASN B	186	27.452	90.450	2.483	1.00	19.98
	ATOM	4020	CA	ASN B	186	28.580	89.570	2.713	1.00	16.29
	ATOM	4021	СВ	ASN E	186	29.722	90.269	3.460	1.00	19.11
	ATOM	4022	CG	ASN E	3 186	30.457	91.254	2.549	1.00	22.13
20	MOTA	4023	OD1	ASN E	3 186	30.227	91.277	1.334	1.00	21.39
	MOTA	4024	ND2	ASN F	3 186	31.353	92.064	3.117	1.00	19.64
	ATOM	4025	С	ASN F	3 186	28.178	88.230	3.283	1.00	11.95
	MOTA	4026	0	ASN I	3 186	29.030	87.417	3.624	1.00	15.32
	MOTA	4027	N	LEU 1	в 187	26.875	87.998	3.326	1.00	13.26
25	ATOM	4028	CA	LEU	B 187	26.277	86.738	3.794	1.00	17.80
	ATOM	4029	CB	LEU	В 187	25.173	87.001	4.838	1.00	16.02
	ATOM	4030	CG	LEU	в 187	25.565	87.835	6.061	1.00	18.73
	MOTA	4031	CD	1 LEU	В 187	24.335	88.161	6.902	1.00	14.44
	MOTA	4032	CD	2 LEU	В 187	26.621	87.103	6.875	1.00	15.90
30	ATOM	4033	C	LEU	в 187	25.650	85.977	2.609	1.00	20.22
	ATOM	4034	0	LEU	B 187	24.612	86.383	2.070	1.00	22.29
	ATOM	4035	S N	LEU	B 188	26.283	84.882	2.220	1.00	23.27
	MOTA	4036	5 CA	LEU	B 188	25.803	3 84.063	1.112	1.00	25.98
	ATOM	4037	7 CE	LEU	B 188	26.98	3 83.456	0.343	1.00	24.19
35	ATOM	4038	3 CG	LEU	в 188	28.09	1 84.426	-0.041	1.00	22.57

	ATOM	4039	CD1	LEU	В	188	29.300	83.683	-0.584	1.00	23.24
	ATOM	4040	CD2	LEU	В	188	27.582	85.467	-1.024	1.00	23.33
	ATOM	4041	C	LEU	В	188	24.909	82.949	1.596	1.00	28.54
	ATOM	4042	0	LEU	В	188	25.114	82.411 .	2.687	1.00	31.17
5	ATOM	4043	N	LEU	В	189	23.934	82.590	0.768	1.00	29.77
	ATOM	4044	CA	LEU	В	189	23.025	81.517	1.098	1.00	30.54
	MOTA	4045	СВ	LEU	В	189	21.679	82.046	1.587	1.00	30.11
	MOTA	4046	CG	LEU	В	189	21.668	83.354	2.349	1.00	27.86
	MOTA	4047	CD1	ΓĖΩ	В	189	20.296	84.000	2.226	1.00	28.53
10	ATOM	4048	CD2	LEU	В	189	22.030	83.105	3.810	1.00	29.39
	ATOM	4049	C	LEU	B	189	22.749	80.615	-0.095	1.00	33.95
•	ATOM	4050	0	LEU	В	189	22.855	81.023	-1.261	1.00	32.29
	ATOM	4051	N	ASP	В	190	22.306	79.412	0.237	1.00	36.30
	MOTA	4052	CA	ASP	В	190	21.893	78.423	-0.726	1.00	38.55
15	ATOM	4053	СВ	ASP	В	190	22.470	77.046	-0.364	1.00	39.02
	ATOM	4054	CG	ASP	В	190	22.338	76.020	-1.487	1.00	40.50
	ATOM	4055	OD1	ASP	Ŗ	190	23.107	75.033	-1.486	1.00	39.94
	ATOM	4056	OD2	ASP	В	190.	21.459	76.197	-2.360	1.00	41.85
	ATOM	4057	С	ASP	В	190	20.362	78.387	-0.691	1.00	40.13
20	ATOM	4058	0	ASP	В	190	19.772	78.016	0.334	1.00	38.56
	MOTA	4059	N .	PRO	В	191	19.697	78.791	-1.804	1.00	41.84
	ATOM	4060	CD	PRO	В	191 .	20.326	79.259	-3.057	1.00	43.11
	ATOM	4061	CA	PRO	В	191	18.229	78.814	-1.894	1.00	43.03
	ATOM	4062	CB	PRO	В	191	17.996	78.792	-3.405	1.00	43.46
25	ATOM	4063	CG	PRO	B	191	19.154	79.557	-3.957	1.00	43.83
	ATOM	4064	С	PRO	В	191	17.635	77.579	-1.236	1.00	42.98
	ATOM	4065	0	PRO	В	191 .	16.719	77.665	-0.426	1.00	44.87
	MOTA	4066	N	ASP	В	192	18.217	76.442	-1.558	1.00	43.24
	MOTA	4067	CA,	ASP	В	192	17.829	75.169	-0.982	1.00	42.75
30	ATOM	4068	CB	ASP	В	192	17.737	74.090	-2.079	1.00	43.62
	MOTA	4069	CG	ASP	В	192	17.232	74.624	-3.418	1.00	44.29
	ATOM	4070	OD1	ASP	В	192	16.060	75.053	-3,487	1.00	43.96
	MOTA	4071	OD2	ASP	В	192	18.011	74.613	-4.397	1.00	46.05
	MOTA	4072	С	ASP	В	192	18.909	74.808	0.035	1.00	42.02
35	ATOM	4073	0	ASP	В	192	20.044	75.256	-0.100	1.00	42.79

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	ATOM	4074	N	THR B 193	18.570	74.035	1.056	1.00 39.71
	ATOM .	4075	CA	THR B 193	19.551	73.668	2.091	1.00 38.55
	ATOM	4076	CB	THR B 193	20.934	73.269	1.519	1.00 38.09
	ATOM	4077	OG1	THR B 193	21.839	74.363	1.479	1.00 37.67
5	ATOM	4078	CG2	THR B 193	20.899	72.623	0.148	1.00 39.30
	ATOM	4079	С	THR B 193	19.679	74.755	3.174	1.00 36.88
	MOTA	4080	0	THR B 193	20.018	74.452	4.312	1.00 37.44
	ATOM	4081	N	ALA B 194	19.381	76.008	2.811	1.00 34.97
	MOTA	4082	CA	ALA B 194	19.426	77.149	3.739	1.00 33.98
10	MOTA	4083	СВ	ALA B 194	18.427	76.970	4.874	1.00 34.13
	ATOM	4084	С	ALA B 194	20.814	77.419	4.307	1.00 33.03
	ATOM	4085	0	ALA B 194	20.951	78.183 _.	5.266	1.00 33.38
	MOTA	4086	N	VAL B 195	21.839	76.811	3.718	1.00 29.95
	ATOM ·	4087	CA	VAL B 195	23.201	77.016	4.182	1.00 25.72
15	MOTA	4088	СВ	VAL B 195	24.183	76.067	3.461	1.00 25.44
	MOTA	4089	CG1	VAL B 195	25.621	76.564	3.537	1.00 24.29
	ATOM	4090	CG2	VAL B 195	24.068	74.657	4.022	1.00 21.03
	ATOM	4091	С	VAL B 195	23.620	78.476	3.999	1.00 25.93
	MOTA	4092	0	VAL B 195	23.219	79.125	3.023	1,00 26.83
20	ATOM	4093	N	LEU B 196	24.420	78.985	4.950	1.00 22.33
	MOTA	4094	CA	LEU B 196	24.908	80.362	4.917	1.00 18.44
	MOTA	4095	CB	LEU B 196	24.288	81.214	6.042	1.00 21.00
	MOTA	4096	CG	LEU B 196	24.668	82.713	6.079	1.00 19.92
	MOTA	4097	CD1	L LEU B 196	23.587	83.533	6.760	1.00 19.76
25	ATOM	4098	CD	2 LEU B 196	26.010	82.931	6.765	1.00 21.62
	ATOM	4099	С	LEU B 196	26.412	80.376	5.025	1.00 18.31
	MOTA	4100	0	LEU B 196	27.000	79.602	5.776	1.00 18.56
•	MOTA	4101	И	LYS B 197	27.048	81.258	4.278	1.00 17.76
	MOTA	4102	CA	LYS B 197	28.486	81.361	4.322	1.00 16.84
30	MOTA	4103	CB	LYS B 197	29.134	80.556	3.207	1.00 20.50
	ATOM	4104	CG	LYS B 197	28.966	79.050	3.363	
•	MOTA	4105	CD	LYS B 197	29.577	78.316	2.188	1.00 21.22
	ATOM	4106	CE	LYS B 197	29.875	76.872	2.525	
	ATOM	4107	NZ	LYS B 197	29.618	75.983	1.362	
35	ATOM	4108	3 C	LYS B,197	28.918	82.804	4.260	1.00 18.70

	ATOM	4109	0	LYS E	3	197	28.379	83.601	3.473	1.00	20.29
	ATOM	4110	N	LEU E	3	198	29.884	83.124	5.126	1.00	19.30
	ATOM	4111	CA	LEU H	3	198	30.468	84.440	5.282	1.00	18.67
	ATOM	4112	СВ	LEU I	В	198	31.199	84.487	6.643	1.00	19.83
5	ATOM	4113	CG	LEU I	В	198	31.049	85.752	7.499	1.00	19.27
	ATOM	4114	CD1	LEU I	В	198	32.200	85.856	8.496	1.00	15.42
	ATOM	4115	CD2	LEU I	В	198	30.983	86.993	6.634	1.00	12.11
	ATOM	4116	С	LEU I	В	198	31.497	84.641	4.186	1.00	18.53
	ATOM	4117	0	LEU I	В	198	32.247	83.721	3.866	1.00	16.63
10	ATOM	4118	N	CYS I	В	199	31.545	85.837	3.611	1.00	18.83
	MQTA	4119	CA	CYS I	В	199	32.509	86.077	2.551	1.00	19.58
	ATOM	4120	СВ	CYS	В	199	31.850	85.881	1.176	1.00	14.83
	MOTA	4121	SG	CYS	В	199	30.667	87.171	0.756	1.00	21.79
	ATOM	4122	С	CYS	В	199	33.114	87.461	2.646	1.00	19.09
15	MOTA	4123	0	CYS	В	199 .	32.754	88.250	3.519	1.00	18.83
	ATOM	4124	N	ASP	В	200	34.040	87.729	1.713	1.00	18.38
	ATOM	4125	CA	ASP	В	200	34.745	88.981	1.604	1.00	15.12
	ATOM	4126	CB	ASP	В	200	33.819	90.129	1.230	1.00	10.15
	MOTA	4127	CG	ASP	В	200	34.584	91.400	0.934	1.00	9.23
20	ATOM	4128	OD1	ASP	В	200	33.950	92.454	0.818	1.00	18.68
	ATOM	4129	OD2	ASP	В	200	35.824	91.345	0.819	1.00	17.92
	MOTA	4130	С	ASP	В	200	35.548	89.290	2.856	1.00	18.42
	MOTA	4131	0	ASP	В	200	35.082	89.992	3.757	1.00	18.47
	MOTA	4132	N	PHE	В	201	36.758	88.756	2.879	1.00	19.43
25	MOTA	4133	CA	PHE	В	201	37.690	88.932	3.970	1.00	20.67
	MOTA	4134	CB	PHE	В	201	38.359	87.588	4.287	1.00	19.84
	MOTA	4135	CG	PHE	В	201	37.461	86.667	5.077	1.00	20.16
	MOTA	4136	CD1	PHE	В	201	36.402	86.009	4.467	1.00	20.40
•	MOTA	4137	CD2	PHE	В	201	37.665	86.475	6.446	1.00	20.19
30	MOTA	4138	CE1	PHE	В	201	35.560	85.184	5.201	1.00	21.68
	MOTA	4139	CE2	PHE	В	201	36.834	85.649	7.185	1.00	18.96
	MOTA	4140	CZ	PHE	В	201	35.780	85.005	6.568	1.00	22.32
	ATOM	4141	C	PHE	В	201	38.720	90.014	3.634	1.00	21.02
	MOTA	4142	0	PHE	B	201	39.811	90.034	4.177	1.00	22.62
35	ATOM	4143	N	GLY	В	202	38.337	90.924	-2.730	1.00	23.59

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	ATOM	4144	CA	GLY B 202	39.206	92.015	2.313	1.00 24.29
	ATOM	4145	С	GLY B 202	39.410	93.093	3.372	1.00 23.17
	ATOM	4146	0	GLY B 202	40.401	93.819	3.342	1.00 23.40
	ATOM	4147	N	SER B 203	38.491	93.197	4.315	1.00 25.53
5	ATOM	.4148	CA	SER B 203	38.617	94.189	5.390	1.00 24.92
	ATOM	4149	СВ	SER B 203	37.283	94.897	5.589	1.00 25.38
	MOTA	4150	OG	SER B 203	37.015	95.804	4.543	1.00 27.73
	ATOM	4151	С	SER B 203	39.006	93.516	6.708	1.00 25.45
	MOTA	4152	0	SER B 203	39.035	94.168	7.750	1.00 28.67
10	ATOM	4153	N	ALA B 204	39.242	92.202	6.663	1.00 24.63
	MOTA	4154	CA	ALA B 204	.39.564	91.396	7.847	1.00 24.22
	MOTA	4155	- CB	ALA B 204	39.383	89.912	7.551	1.00 21.47
	MOTA	4156	С	ALA B 204	40.957	91.672	8.416	1.00 24.85
	MOTA	4157	0	ALA B 204	41.871	92.076	7.695	1.00 20.84
15	MOTA	4158	N	LYS B 205	41.116	91.461	9.737	1.00 24.29
	ATOM	4159	CA	LYS B 205	42.407	91.716	10.369	1.00 24.23
	ATOM	4160	СВ	LYS B 205	42.583	93.216	10.584	1.00 22.03
	ATOM	4161	CG	LYS B 205	44.029	93.655	10.548	1.00 24.61
	MOTA	4162	CD	LYS B 205	44.229	94.953	11.308	1.00 23.18
20 .	ATOM	4163	CE	LYS B 205	45.596	95.010	11.957	1.00 24.28
	ATOM	4164	NZ	LYS B 205	46.307	96.273	11.632	1.00 29.00
	ATOM	4165	С	LYS B 205	. 42.601	90.994	11.704	1.00 25.96
	ATOM	4166	0	LYS B 205	41.662	90.788	12.477	1.00 25.46
	ATOM	4167	N	GLN B 206	43.860	90.671.	11.972	1.00 28.37
25	ATOM	4168	CA	GLN B 206	-44.269	90.032	13.208	1.00 29.42
	MOTA	4169	CB	GLN B 206	45.544	89.230	12.967	1.00 32.05
	ATOM	4170	CG	GLN B 206	45.375	88.117	11.937	1.00 38.78
	MOTA	4171	CD	GLN B 206	45.021	86.772	12.554	1.00 41.77
	ATOM	4172	OE1	GLN B 206	44.861	85.776	11.840	1.00 43.68
30	MOTA	4173	NE2	GLN B 206	44.904	86.731	.13.885	1.00 42.59
	ATOM	4174	С	GLN B 206	44.514	91.112	14.259	1.00 27.78
	MOTA	4175	0	GLN B 206	45.570	91.719	14.299	1.00 27.97
	ATOM	4176	N	LEU B 207	43.508		15.077	1.00 28.77
	MOTA	4177	CA	LEU B 207	43.591	92.401	16.101	1.00 28.47
35	MOTA	4178	CB	LEU B 20	42.215	92.671	16.709	1.00 27.69

	ATOM	4179	CG	LEU	В	207	41.111	93.057	15.727	1.00	29.12
	ATOM	4180	CD1	LEU :	В	207	39.953	93.708	16.463	1.00	27.92
	ATOM	4181	CD2	LEU	В	207	41.649	93.985	14.645	1.00	28.33
	ATOM	4182	C	LEU	В	207	44.591	92.060	17.192	1.00	28.80
5	ATOM	4183	0	LEU :	В	207	44.622	90.934	17.698	1.00	29.81
	MOTA	4184	N	VAL	В	208	45.395	93.054	17.558	1.00	30.07
	MOTA	4185	CA	VAL	В	208	46.393	92.904	18.614	1.00	30.14
	ATOM	4186	СВ	VAL	В	208	47.810	92.530	18.110	1.00	30.08
	MOTA	4187	CG1	VAL	В	208	47.763	91.621	16.885	1.00	31.56
10	ATOM	4188	CG2	VAL	В	208	48.659	93.757	17.849	1.00	32.50
•	ATOM	4189	С	VAL	В	208	46.417	94.153	19.497	1.00	29.58
	MOTA	4190	0	VAL	В.	208	46.334	95.275	18.992	1.00	27.39
	ATOM	4191	N	ARG	В	209	46.487	93.924	20.823	1.00	30.91
	ATOM	4192	CA	ARG	В	209	46.479	94.991	21.849	1.00	31.31
15	ATOM	4193	CB	ARG	В	209	46.964	94.423	23.206	1.00	31.12
	ATOM	4194	CG	ARG	В	209	47.860	95.375	24.011	1.00	29.38
	ATOM	4195	CD	ARG	В	209	47.882	95.037	25.502	1.00	26.82
	ATOM	4196	NE	ARG	В	209	47.812	96.245	26.319	1.00	21.48
	MOTA	4197	CZ	ARG	В	209	46.672	96.767	26.796	1.00	23.43
20	MOTA	4198	NH1	ARG	В	209	45.510	96.124	26.651	1.00	20.48
	ATOM	4199	NH2	ARG	В	209	46.698	97.934	27.434	1.00	25.12
	MOTA	.4.200	С	ARG	В	209	47.319	96.213	21.485	1.00	31.54
	ATOM	4201	0	ARG	В	209	46.815	97.335	21.453	1.00	34.08
	ATOM	4202.	N	GLY	В	210	48.606	96.004	21.280	1.00	32.47
25	ATOM	4203	CA	GLY	В	210	49.494	97.118	20.995	1.00	34.33
	ATOM	4204	C	GLY	В	210	49.109	98.001	19.812	1.00	35.22
	ATOM	4205	0	GLY	В	210	48.892	99.209	19.974	1.00	35.81
	ATOM	4206	N	GLU	В	211	49.097	97.410	18.615	1.00	35.57
	ATOM	4207	CA	GLU	В	211	48.825	98.140	17.371	1.00	32.82
30	ATOM	4208	CB	GLU	В	211	49.240	97.316	16.150	100	35.30
	MOTA	4209	CG	GLU	В	211	48.588	95.946	16.085	1.00	37.01
	MOTA	4210	CD	GLU	В	211	49.189	95.054	15.011	1.00	38.55
	ATOM	4211	OE1	GLU	В	211	50.326	94.560	15.212	1.00	38.76
	ATOM	4212	OE2	GLU	В	211	48.517	94.842	13.977	1.00	36.23
35	ATOM	4213	.C	GLU	В	211	47.402	98.656	17.212	1:00	29.12

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	MOTA	4214	0	GLU B 211	46.431	97.909	17.298	1.00 3	30.00
	ATOM	4215	N	PRO B 212	47.273	99.957	16.933	1.00 2	26.97
	ATOM	421.6	CD	PRO B 212	48.391	100.908	16.785	1.00 2	26.49
	ATOM	4217	CA	PRO B 212	45.980	100.590 .	16.707	1.00 2	26.42
5	ATOM	4218	CB	PRO B 212	46.305	102.081	16.805	1.00	26.02
	MOTA	4219	CG	PRO B 212	47.723	102.187	16.374	1.00	25.87
	ATOM .	4220	С	PRO B 212	45.430	100.254	15.306	1.00	25.79
	MOTA	4221	0	PRO B 212	46.169	99:812	14.422	1.00	25.35
	MOTA	4222	N	ASN B 213	44.131	100.459	15.130	1.00	24.87
10	MOTA	4223	CA	ASN B 213	43.445	100.187	13.875	1.00	25.11
	MOTA	4224	CB	ASN B 213	42.583	98.934	13.998	1.00	25.01
	MOTA	4225	CG	ASN B 213	43.400	97.703	14.319	1.00	27.74
	MOTA	4226	OD1	ASN B 213	44.306	97.333	13.570	1.00	29.67
	ATOM	4227	ND2	ASN.B 213	43.092	97.063	15,443	1.00	27.23
15	ATOM	4228	С	ASN B 213	42.579	101.370	13.491	1.00	24.44
	ATOM	4229	0	ASN B 213	42.169	102.145	14.355	1.00	22.83
	ATOM	4230	N	VAL B 214	42.304	101.515	12.188	1.00	24.44
	MOTA	4231	CA	VAL B 214	41.482	102.630	11.711	1.00	21.41
	MOTA	4232	CB	VAL B 214	41.536	102.812	10.165	1.00	24.20
20	ATOM	4233	CG1	VAL B 214	42.975	102.952	9.698	1.00	21.35
	ATOM	4234	CG2	VAL B 214	40.841	101.659	9.444	1.00	20.54
	ATOM	4235	С	VAL B 214	40.041	102.501	12.192	1.00	19.64
	ATOM	4236	0	VAL B 214	39.511	101.399	12.323	1.00	20.17
	ATOM	4237	N	SER B 215	39.421	103.636	12.474	1.00	20.26
25	MOTA	4238	CA	SER B 215	38.046	103.670	12.967	1.00	20.21
	MOTA	4239	CB	SER B 215	37.862	2 104.860	13.907	1.00	21.10
	ATOM	4240	OG	SER B 215	38.487	7 106.017	13.378	1.00	23.88
	ATOM	4241	С	SER B 215	36.995	5 103.698	11.841	1.00	20.47
	ATOM	4242	Ο.	SER B 215	35.899	9 103.162	11.999	1.00	19.45
30	MOTA	4243	N	PTR B 216	37.323	3 104.316	10.707	1.00	22.87
	MOTA	4244	CA	PTR B 216	36.37	8 104.370	9.582	1.00	23.82
	ATOM	4245	CB	PTR B 216	36.68	3 105.571	8.654	1.00	24.62
	ATOM	4246	CG	PTR B 216	35.50	7 106.017	7.799	1.00	24.52
	MOTA	4247	.CD	1 PTR B 216	34.79	8 107.173	8.107	1.00	25.84
35	MOTA	4248	CE	1 PTR B 216	33.72	2 107.591	7.327	1.00	27.22

	ATOM	4249	CD2	PTR B	3 ,	216	35104	105.283	6.675	1.00	25.91
	.ATOM	4250	CE2	PTR E	3 2	216	34.025	105.691	5.890	1.00	27.15
	ATOM	4251	CZ	PTR E	3 2	216	33.334	106.847	6.219	1.00	26.61
	ATOM	4252	он .	PTR E	3 2	216	32.261	107.279	5.450	1.00	26.46
5	ATOM	4253	С	PTR E	3 2	216	36.445	103.053	8.811	1.00	23.08
	ATOM	4254	0	PTR E	3 2	21,6	37.208	102.916	7.869	1.00	24.94
	ATOM	4255	P	PTR E	3 2	216	31.041	106.344	5.227	1.00	27.03
	ATOM	4256	01P	PTR E	3 3	216	30.362	106.877	3.942	1.00	30.42
	ATOM	4257	02P	PTR E	3 :	216	30.099	106.633	6.418	1.00	28.23
10	ATOM	4258	03P	PTR E	3 :	216	31.426	104.917	5.114 .	1.00	24.51
	ATOM	4259	N	ILE E	3 :	217	35.749	102.053	9.346	1.00	24.80
	ATOM	4260	CA	ILE E	3 2	217	35.641	100.783	8.656	1.00	23.98
	ATOM	4261	CB	ILE E	3	217	36.542	99.693	9.287	1.00	26.25
	MOTA	4262	CG2	ILE E	3 .	217	37.778	99.450	8.438	1.00	25.26
1:5	ATOM	4263	CG1	ILE E	3	217	36.953	100.051	10.708	1.00	26.90
	MOTA	4264	CD1	ILE E	3	217	37.119	98.845	11.613	1.00	27.85
	ATOM	4265	C	ILE E	3	217	34.195	100.382	8.691	1.00	24.40
	MOTA	4266	0	ILE E	3	217	33.361	101.080	9.276	1.00	26.29
	ATOM	4267	N	CYS F	3	218	33.911	99.263	8.073	1.00	24.77
20	MOTA	4268	CA	CYS I	3	218	32.541	98.748	8.030	1.00	23.40
	MOTA.	4269	CB	CYS F	3	218	31.965	98.740	9.450	1.00	23.30
•	ATOM	4270	SG	CYS I	В	218	32.745	97.535	10.578	1.00	26.72
	ATOM	4271	С	CYS F	В	218	31.653	99.526	7.070	1.00	23.74
	ATOM .	4272	0	CYS I	В	218	32.051	100.535	6.510	1.00	27.68
25	ATOM	4273	N	SER I	В	219	30.463	99.027	6.853	1.00	22.47
	MOTA	4274	CA	SER I	В	219	29.481	99.745	6.088	1.00	22.56
	ATOM	. 4275	CB	SER I	В	219	28.517	98.836	5.344	1.00	16.39
	ATOM	4276	OG	SER 1	В	219	27.433	99.582	4.804	1.00	24.70
	ATOM	4277	С	SER	В	219	28.732	100.597	7.092	1.00	23.73
30	ATOM	4278	0	SER !	В	219	28.194	100.091	8.082	1.00	26.17
	ATOM	4279	N	ARG	В	220	28.678	101.890	6.835	1.00	22.97
	MOTA	4280	CA	ARG	В	220	28.046	102.841	7.732	1.00	23.82
	ATOM	4281	CB	-ARG	В	220	27.485	104.019	6.956	1.00	22.63
	ATOM	4282	CG	ARG	В	220	26.816	105.032	7.862	1.00	23.19
35	ATOM	4283	CD	ARG	В	220	26.068	106.069	7.070	1.00	21.58

	ATOM	4284	NE	ARG B	3 22	20 .		26.939	10	06.750	6.124	1.00	22.96	
	ATOM	4285	CZ	ARG E	3 22	20		26.515	10	07.289	4.984	1.00	23.07	
	MOTA	4286	NH1	ARG E	3 22	20		25.240	10	07.221	4.634	1.00	20.87	
	ATOM	4287	NH2	ARG E	3 22	20		27.377	10	07.897	4.195	1.00	24.87	
5	ATOM	4288	С	ARG E	3 22	20	•	26.952	1	02.240	8.617	1.00	24.57	
	ATOM .	4289	0	ARG E	3 2	2 0		27.083	1	02.186	9.840	1.00	29.08	
	ATOM	4290	N .	TYR E	3 2	21		25.869	1	01.778	7.997	1.00	22.44	
	ATOM	4291	CA	TYR F	3 2	21		24.708	1	01.225	8.682	1.00	21.21	
	ATOM	4292	СВ	TYR F	3 2	21		23.732	1	00.619	7.671	1.00	22.74	
10	ATOM	4293	CG	TYR I	в 2	21		23.028	1	01.592	6.747	1.00	25.19	
	ATOM	4294	CD1	TYR I	B 2	21		22.137	1	01.122	5.786	1.00	26.74	
	ATOM	4295	CE1	TYR I	в 2	21		21.484	1	01.981	4.921	1.00	29.14	
	ATOM	4296	CD2	TYR I	в 2	21	•	23.248	1	.02.959	6.818	1.00	26.22	
	ATOM	4297	CE2	TYR	в 2	21		22.599	1	.03.830	5.960	1.00	28.68	
15	MOTA	4298	CZ	TYR	B 2	221		21.717	1	.03.334	5.011	1.00	29.87	
	ATOM	4299	ОН	TYR	B 2	221		21.076	5 1	.04.193	4.154	1.00	28.44	
	ATOM	4300	С	TYR	B 2	221		25.025	5 1	100.169	9.761	1.00	20.80	
	MOTA	4301	0	TYR	В 2	221		24.239	9 1	100.001	10.695	1.00	21.60	
	MOTA	4302	N	TYR	B 2	222		26.116	5	99.433	9.585	1.00	16.82	
20	ATOM	4303	CA	TYR	B 2	222		26.512	2	98.341	10.477	1.00	17.54	
	MOTA	4304	СВ	TYR	В 2	222		26.73	4	97.073	9.611	.1.00	17.40	
	MOTA	4305	CG	TYR	В 2	222		25.63	4	96.916	8.575	1.00	19.92	
	MOTA	4306	CD1	TYR	В 2	222		24.51	7	96.131	8.836	• .	19.27	
	MOTA	. 4307	CE1	TYR	В	222		23.46	9	96.062	7.943	1.00	21.70	
25	ATOM	4308	CD2	2 TYR	В	222		25.67	2	97.628	7.374	1.00	21.19	!
	ATOM	4309	CE	2 TYR	В	222		24.62	8	97.549	6.463		20.78	
	MOTA	4310	CZ	TYR	В	222		23.52	8	96.770	6.759	1.0	0 21.97	,
	ATOM	4311	ОН	TYR	В	222		22.46	6	96.725	5.892		0 21.65	
	ATOM	4312	C	TYR	В	222		27.76	4	98.666	11.292		0 15.94	
30	ATOM	4313	0	TYR	В	222		28.40	9 .	97.769	11.841		0 18.58	
	MOTA	4314	N	ARG	В	223		28.10)5	99.936	11.356	1.0	0 15.02	2
	MOTA	4315	CA	ARG	В	223		29.28	35	100.393	12.079		0 17.28	
	ATOM	4316	CE	ARG	В	223		29.76	54	101.686	11.436		0 14.6	
	ATOM	4317	CG	ARG	B	223				102.114			0 14.12	
35	ATOM	4318	CE	ARG	B	223		31.53	35	103.403	11.175	5 1.0	00 18.43	2

	ATOM	4319	NE	ARG E	3	223	32.044	103.122	9.835	1.00	20.42
	ATOM	4320	CZ	ARG E	3	223	31.654	103.746	8.720	1.00	20.83
	MOTA	4321	NH1	ARG E	3	223	30.909	104.835	8.767	1.00	17.04
•	MOTA	4322	NH2	ARG E	3	223	32.062	103.282	7.546	1.00	21.59
5 -	ATOM	4323	С	ARG I	3	223	28.990	100.634	13.585	1.00	16.29
	ATOM	4324	0	ARG E	3	223 .	28.024	101.318	13.934	1.00	16.79
	ATOM	4325	N	ALA E	3	224	29.837	100.063	14.438	1.00	17.91
	ATOM	4326	CA	ALA E	3	224	29.722	100.177	15.913	1.00	19.04
	ATOM	4327	CB	ALA F	3	224	30.712	99.232	16.570	1.00	16.46
10	ATOM	4328	С	ALA E	3	224	29.966	101.607	16.397	1.00	18.94
	ATOM	4329	0	ALA E	3	224	30.870	102.279	15.916	1.00	21.70
	ATOM	4330	N	PRO E	3	225	29.183	102.079	17.383	1.00	21.63
	ATOM	4331	ĊD	PRO 'E	3	225	28.120	101.321	18.062	1.00	23.65
	ATOM	4332	CA	PRO I	3	225	29.315	103.440	17.954	1.00	22.23
15	ATOM	4333	CB	PRO E	3	225	28.444	103.404	19.221	1.00	23.95
	ATOM	4334	CG	PRO F	3	225	28.089	101.965	19.424	1.00	22.74
	ATOM	4335	С	PRO E	3	225 ·	30.743	103.811	18.315	1.00	20.39
	MOTA	4336	0	PRO ·	3	225	31.152	104.962	18.150	1.00	22.02
	ATOM	4337	N	GLU F	3	226	31.501	102.832	18.797	1.00	19.06
20	MOTA	4338	CA	GLU F	3	226	32.898	103.041	19.179	1.00	19.14
	ATOM	4339	CB	GLU F	3	226	33.450	101.789	19.851	1.00	18.75
	ATOM	4340	CG	GLU I	3.	226	32.562	100.561	19.645	1.00	20.23
	MOTA	4341	CD	GLU I	3	226	33.352	99.289	19.603	1.00	17.38
	ATOM	4342	OE1	GLU 1	3	226	32.736	98.213	19.618	1.00	19.90
25	ATOM	4343	OE2	GLU I	3	226	34.598	99.368	19.552	1.00	24.74
	ATOM	4344	С	GLU I	3	226	33.746	103.423	17.963	1.00	20.82
	ATOM	4345	0	GLU I	В	226	34.666	104.248	18.066	1.00	20.13
	ATOM	4346	N	LEU 1	В	227	33.408	102.851	16.800	1.00	19.41
	ATOM	4347	CA	LEU 1	В	227	34.110	103.184	15.556	1.00	19.05
30	MOTA	4348	CB	LEU 1	В	227	33.629	102.290	14.407	1.00	16.10
	MOTA	4349	CG	LEU	В	227	34.416	101.013	14.147	1.00	15.05
	MOTA	4350	CD1	LEU	В	227	35.803	101.042	14.756	1.00	12.73
	MOTA	4351	CD2	LEU	В	227	33.641	99.800	14.580	1.00	14.58
	MOTA	4352	С	LEU	В	227	33.779	104.624	15.220	1.00	14.97
35	ATOM	4353	0	LEU	В	227	34.655	105.405	14.906	1.00	20.12

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	MOTA	4354	N	ILE B 228	32.496 104.961	15.340	1.00 17.59
	MOTA	4355	CA	ILE B 228	31.993 106.311	15.103	1.00 18.11
	MOTA	4356	CB	ILE B 228	30.471,106.365	15.223	1.00 18.51
	ATOM	4357	CG2	ILE B 228	29.947 107.738	14.812	1.00 21.29
5	ATOM	4358	CG1	ILE B 228	29.862 105.261	14.349	1.00 18.14
	MOTA	4359	CD1	ILE B 228	28.353 105.347	14.185	1.00 16.84
	MOTA	4360	C	ILE B 228	32.678 107.310	16.049	1.00 23.42
	ATOM	4361	0	ILE B 228	32.848 108.489	15.716	1.00 24.97
	ATOM .	4362	N	PHE B 229 '	33.167 106.795	17.182	1.00 23.68
10	ATOM .	4363	CA	PHE B 229	33.958 107.584	18.111	1.00 25.34
	MOTA	4364	CB	PHE B 229	33.707 107.151	19.578	1.00 22.49
	MOTA	4365	CG	PHE B 229	32.480 107.775	20.225	1.00 19.47
	MOTA	4366	CD1	PHE B 229	31.276 107.093	20.272	1.00 17.35
	MOTA	4367	CD2	PHE B 229	32.534 109.048	20.782	1.00 20.35
15	MOTA	4368	CE1	PHE B 229	30.157 107.659	20.852	1.00 17.59
	ATOM	4369	CE2	2 PHE B 229	31.415 109.619	21.365	1.00 17.04
•	ATOM	4370	CZ	PHE B 229	30.225 108.923	21.398	1.00 18.69
	ATOM	4371	C.	PHE B 229	35.402 107.294	17.669	1.00 26.92
	ATOM	4372	0	PHE B 229	35.636 106.318	16.975	1.00 29.38
20	MOTA	4373	N .	GLY B 230	36.364 108.125	17.992	1.00 28.35
	MOTA	4374	CA	GLY B 230	. 37.725 107.851	17.493	1.00 26.41
	ATOM	4375	C	GLY B 230	38.364 106.514	17.891	1.00 25.16
	ATOM	4376	0	GLY B 230	39.580 106.387	17.800	1.00 24.78
	MOTA	4377	N	ALA B 231	37.577 105.530	18.348	1.00 25.97
25	MOTA	4378	CA	ALA B 231	38.134 104.234	18.788	1.00 26.04
	MOTA	4379	CB	ALA B 231	37.065 103.275	19.280	1.00 26.83
	ATOM	4380	C	ALA B 231	39.050 103.575	17.767	1.00 26.99
	MOTA	4381	. 0	ALA B 231	38.628 103.158		1.00 27.04
	MOTA	4382	2 N	THR B 232	40.303 103.485		1.00 26.36
30	MOTA	4383	3 CP	THR B 232	41.349 102.893	17.346	
	MOTA	4384	CE	3 THR B 232	42.460 103.926	17.200	1.00 26.18
	ATOM	4385	5 00	G1 THR B 232	43.518 103.434	16.410	
	ATOM	438	6	32 THR B 232	43.039 104.388	18.520	
	MOTA	438	7 C	THR B 232	41.889 101.622		
35	MOTA	438	8 0	THR B 232	42.769 100.948	3 17.476	1.00 25.89

•		ATOM	4389 ·	N	ASP F	3 233	41.361	101.306	19.206	1.00 25.99	
		ATOM	4390	CA	ASP E	3 233	41.795	100.134	19.967	1.00 24.56	
•		ATOM	4391	CB	ASP E	3 233	42.508	100.609	21.257	1.00 28.62	
		MOTA	4392	ÇG	ASP E	3 233	42.360	99.698	22.462	1.00 30.06	
	5	ATOM	4393	OD1	ASP E	3 233	41.434	99.937	23.262;	1.00 34.24	
		MOTA	4394	OD2	ASP E	3 233	43.170	98.751	22.607	1.00 31.50	
		MOTA	4395	С	ASP E	3 233	40.642	99.138	20.217	1.00 23.91	
		ATOM	4396	0	ASP E	3 233	40.721	98.264	21.080	1.00 26.44	
		ATOM	4397	N	TYR E	3 234	39.582	99.258	19.426	1.00 22.91	
	10	ATOM	4398	CA	TYR E	3 234	38.416	98.374	19.516	1.00 20.38	
		ATOM	4399	CB ·	TYR F	3 234	37.380	98.748	18.452	1.00 23.38	
		MOTA	4400	CG	TYR E	3 234	37.960	98.779	17.059	1.00 22.55	
		MOTA	4401	CD1	TYR E	3 234	38.028	97.621	16.292	1.00 24.15	
		MOTA	4402	CE1	TYR F	3 234	38.586	.97.634	15.026	1.00 24.83	
	15	ATOM	4403	CD2	TYR I	3 234	38.463	99.958	16.524	1.00 24.39	
		MOTA	4404	CE2	TYR I	3 234	39.020	99.987	15.256	1.00 25.51	
		ATOM	4405	CZ	TYR I	3 234	39.079	98.816	14.513	1.00 26.35	
		MOTA	4406	ОН	TYR F	3 234	39.637	98.829	13.264	1.00 28.21	
		MOTA	4407	C	TYR I	3 234	38.799	96.894	19.394	1.00 16.79	
	20	ATOM	4408	0	TYR I	3 234	39.955	96.553	19.144	1.00 19.38	
		MOTA	4409	N	THR I	3 235	37.811	96.028	19.600	1.00 13.77	
		MOTA	4410	CA	THR I	3 235	37.994	94.578	19.559	1.00 15.58	
•		ATOM	4411	CB	THR. I	3 235	37.720	93.997	20.961	1.00 11.90	
		ATOM.	4412	OG1	THR 1	3 235	36.323	93.922	21.190	1.00 11.51	
	25	ATOM	441,3	CG2	THR 1	3 235 .	38.331	94.801	22.094	1.00 14.31	
		MOTA	4414	C	THR 1	3 235	37.020	93.927	18.573	1.00 14.16	
		ATOM	4415	0	THR	B 235	36.270	94.612	17.896	1.00 16.98	
		ATOM	4416	N	SER :	B 236	37.034	92.597	18.544	1.00 17.59	
		ATOM	4417	CA	SER	В 236	36.164	91.783	17.682	1.00 18.69	
	30	MOTA	4418	СВ	SER	В 236	36.558	90.315	17.749	1.00 18.45	
		ATOM	4419	OG	SER	B 236	37.774	90.092	17.041	1.00 24.22	
		MOTA	4420	С	SER	В 236	34.681	91.961	17.979	1.00 20.02	
		MOTA	4421	0	SER	в 236	33.818	91.472	17.225	1.00 20.26	
		MOTA	4422	N	SER	B 237	34.377	92.686	19.053	1.00 18.28	
	35	MOTA	4423	CA	SER	В 237	32.998	92.964	19.428	1.00 14.71	
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	ATOM	4424	CB.	SER B	237	32.950	93.669	20.791	1.00 1	.5.53
	MOTA	4425	OG	SER B	237	33.890	94.728	20.825	1.00 1	6.04
	ATOM	4426	С	SER B	237	32.313	93.853	18.388	1.00 1	12.17
	ATOM	4427	0	SER B	237	31.092	93.914	18.335	1.00	8.50
5	ATOM	4428	N	ILE B	238	33.086	94.551	17.552	1.00	14.47
	ATOM	4429	ĊА	ILE B	238	32.436	95.390	16.518	1.00	16.29
	MOTA	4430	CB	ILE B	238	33.426	96.260	15.714	1.00	16.74
	MOTA	4431	CG2	ILE B	238	34.121	97.275	16.622	1.00	16.15
	MOTA	4432	CG1	ILE B	238	34.444	95.401	14.951	1.00	13.48
10	MOTA	4433	CD1	ILE B	238	35.264	96.191	13.953	1.00	13.12
	ATOM	4434	С	ILE B	238	31.608	94.500	15.573	1.00	14.21
	ATOM	4435	0	ILE E	238	30.516	94.872	15.157	1.00	18.18
	MOTA	4436	N	ASP E	3 239 .	32.119	93.296	15.293	1.00	15.25
	ATOM	4437	CA	ASP E	3 239	31.423	92.306	14.442	1.00	15.37
15	ATOM	4438	СВ	ASP F	3 239	32.281	91.036	14.263	1.00	13.37
	MOTA	4439	CG	ASP H	3 239	33.405	91.194	13.273	1.00	13.63
	ATOM	4440	OD1	ASP I	3 239	33.409	92.200	12.542	1.00	14.70
	MOTA	4441	OD2	ASP I	B 239	34.298	90.306	13.236	1.00	16.99
•	MOTA	4442	C	ASP 1	B 239	30.089	91.908	15.064	1.00	16.77
20	MOTA	4443	0	ASP 3	B 239	29.076	91.742	14.355	1.00	16.53
	MOTA	4444	Ŋ	VAL	в 240	30.072	91.754	16.416		15.89
	ATOM	4445	CA	VAL	B 240	28.829	91.378	17.109	1.00	12.01
•	ATOM	4446	CB	. VAL	В 240	29.046	91.059	18.624	1.00	14.35.
	ATOM	4447	CG	1 VAL	B 240	27.737	91.199	19.387	1.00	9.00
25	MOTA	4448	CG	2 VAL	B 240	29.604	89.650	•	1.00	13.00
	ATOM	4449	С	VAL	В 240	27.787	92.464	16.952	1.00	8.73
	ATOM	4450	0	VAL	B 240	26.603	92.192	16.799		14.10
	MOTA	4451	N	TRP	B 241	28.227	93.698	16.967		10.49
	MOTA	4452	CA	TRP	B 241	27.303	94.807	16.790		13.99
30	ATOM	4453	CE	TRP	B 241	28,004	96.139	17.103		11.75
	ATOM	4454	t Co	TRP	B 241	27.184	97.333	16.716		12.61
	MOTA	4455	5 CI	2 TRP	B 241	26.34]	98.132	17.564	1.00	18.21
	MOTA	4456	6 CI	E2 TRP	B 241	25.748	99.12			18.68
	ATOM	445	7 CI	E3 TRP	B 241	26.02	7 98.109	18.931		18.35
35	ATOM	445	8 C	D1 TRP	B 241	27.07	4 97.86	7 15.465	1.00	15.24

	MOTA	4459	NE1	TRP	В	241	26.205	98.929	15.473	1.00	18.13
	ATOM -	4460	CZ2	TRP	В	241	24.861	100.078	17.245	1.00	21.75
	MOTA	4461	CZ3	TRP	В	241	25.150	99.051	19.426	1.00	21.43
	MOTA	4462	CH2	TRP	В	241	24.572	100.024.	18.588	1.00	24.55
5	ATOM	4463	С	TRP	В	241	26.728	94.791	15.340	1.00	12.69
	MOTA	4464	0	TRP	В	241	25.543	95.009	15.131	1.00	12.66
	ATOM	4465	N	SER	В	242	27.588	94.505	14.349	1.00	14.14
	MOTA	4466	CA	SER	В	242	27.148	94.435	12.938	1.00	14.63
	ATOM	4467	CB	SER	В	242	28.327	94.072	12.029	1.00	10.79
10	ATOM	4468	OG	SER	В	242	29.311	95.084	12.076	1.00	12.39
	MOTA	4469	С	SER	В	242	26.071	93.386	12.810	1.00	13.69
	ATOM,	4470	0	SER	В	242	24.987	93.650	12.297	1.00	15.83
	MOTA	4471	N	ALA	В	243	26.370	92.194	13.328	1.00	15.65
	ATOM	4472	CA	ALA	В	243	25.426	91.088	13.316	1.00	16.55
15	MOTA	4473	CB	ALA	В	243	26.034	89.868	13.981	1.00	17.84
	MOTA	4474	С	ALA	В	243	24.106	91.483	13.974	1.00	17.41
	ATOM	4475	0	ALA	В	243	23.037	90.993	13.589	1.00	17.38
	MOTA	4476	N	GLY	В	244	24.175	92.403	14.951	1.00	19.03
	MOTA	4477	CA	GLY	В	244	22.957	92.867	15.607	1.00	17.62
20	ATOM	4478	С	GLY	В	244	-22.158	93.748	14.677	1.00	17.92
	MOTA	4479	,O	GLY	В	244	20.942	93.632	14.577	1.00	17.59
	MOTA	4480	N	CYS	В	245	22.854	94.609	13.952	1.00	19.90
	ATOM	4481	CA	CYS	В	245	22.191	95.467	12.974	1.00	19.65
	ATOM	4482	CB	ĊYS	В	245	23.201	96.399	12.318	1.00	19.83
25	ATOM	4483	SG	CYS	В	245	23.913	97.637	13.424	1.00	22.50
•	MOTA	4484 .	С	CYS	В	245	21.537	94.590	11.906	1.00	18.91
	ATOM	4485	0	CYS	В	245	20.475	94.911	11.394	1.00	22.00
	ATOM	4486	N	VAL	В	246	22.178	93.463	11.596	1.00	20.35
	ATOM	4487	CA	VAL	В	246	21.664	92.510	10.606	1.00	20.75
30	MOTA	4488	CB	VAL	В	246	22.680	91.385	10.324	1.00	18.97
	ATOM	4489	CG1	VAL	В	246	22.076	90.328	9.398	1.00	19.70
	ATOM	4490	CG2	VAL	В	246	23.965	91.952	9.752	1.00	19.92
	ATOM	4491	С	VAL	В	246	20.374	91.877	11.094	1.00	22.64
	ATOM	4492	0	VAL	В	246	19.347	91.905	10.400	1.00	26.23
35	ATOM	4493	Ŋ.	LEU	В	247	20.425	91.310	12.308	1.00	22.64
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	ATOM	4494	CA	LEU B	247	19.262	90.672	12.914	1.00 19.95
	ATOM	4495	СВ	LEU B	247	19.630	90.135	14.316	1.00 22.43
	ATOM	4496	CG	LEU B	247	18.486	89.838	15.293	1.00 20.19
	ATOM	4497	CD1	LEU B	247	17.871	91.125	15.811	1.00 22.92
5	ATOM	4498	CD2	LEU B	247	17.428	88.951	14.659	1.00 21.05
	ATOM	4499	С	LEU B	247	18.082	91.632	12.975	1.00 20.28
	ATOM	4500	0	LEU B	247	16.959	91.267	12.620	1.00 21.69
	ATOM	4501	N	ALA B	3 248	18.337	92.864	13.432	1.00 20.15
•	ATOM	4502	CA	ALA B	3 248	17.281	93.873	13.543	1.00 20.23
10	ATOM	4503	СВ	ALA E	3 248.	17.795	95.114	14.261	1.00 17.38
	ATOM	4504	С	ALA E	3 248	16.718	94.230	12.162	1.00 19.28
	ATOM	4505	0	ALA E	3 248	15.507	94.393	11.995	1.00 17.25
	MOTA	4506	N	GLU E	3 249	17.606	94.322	11.171	1.00 21.23
	MOTA	4507	CA	GLU F	B 249	17.186	94.620	9.798	1.00 20.11
15	ATOM	4508	СВ	GLU I	B 249	18.404	94.766	8.867	1.00 22.01
	ATOM	4509	CG	GLU 1	В 249	18.081	95.498	7.573	1.00 24.30
	ATOM	4510	CD	GLU I	В 249	19.266	95.673	6.650	1.00 24.80
	MOTA	4511	OE:	1 GLU	В 249	20.400	95.818	7.144	1.00 25.98
	MOTA	4512	OE:	2 GLU	В 249	19.054	95.684	5.420	1.00 27.86
20	ATOM	4513	С	GLU	B 249	16.229	93.521	9.301	1.00 17.75
	ATOM	4514	Ō	GLU	B 249	15.170	93.808	8.766	1.00 18.76
	ATOM	4515	N	LEU	B 250	16.594	92.262	9.536	1.00 19.74
	MOTA	4516	CA	LEU	B 250	15.762	91.119	9.146	1.00 21.76
	MOTA	4517	CE	LEU	B 250	16.456	89.814	9.498	
25	MOTA	4518	CG	· LEU	B 250	17.846	89.609	8.911	
	MOTA	4519	CI	1 LEU	B 250	18.390	88.246		
	MOTA	4520	CI	02 LEU	в 250	17.816	89.758	•	
	MOTA	4521	С	LEU	B 250	14.372	91.136		_
•	ATOM	4522	0	LEO	B 250	13.395	90.722		Α
30	MOTA	4523	N	LEU	B 251	14.28			
	MOTA	4524	C.	A LEU	B 251	13.01	6 91.63		
	MOTA	4525	S C	B LEU	B 251	13.26	7 91.68		
	ATOM	4526	5 C	G LEU	J В 251	14.09			•
	ATOM	4527	7 C	D1 LEC	J B 251	14.66			
· 35	ATOM	4528	3 C	D2 LEC	J B 251	13.24	4 89.29	1 14.02	9 1.00 23.22

	ATOM	4529	С	LEU I	3	251	12.201	92.866	11.384	1.00	25.00
	ATOM	4530	0	LEU I	3 ·	251 ·	10.976	92.808	11.306	1.00	25.53
	MOTA	4531	И· .	LEU 1	3	252	12.895	93.982	11.191	1.00	27.31
	MOTA	4532	CA	LEU 1	В	252	12.275	95.270	10.862	1.00	28.85
5	MOTA	4533	СВ	LEU 1	3	252	13.247	96.394	11.208	1.00	29.10
	ATOM	4534	CG	LEU 1	В	252	12.820	97.347	12.316	1.00	30.29
•	ATOM	4535	CD1	LEU 1	В	252	13.857	98.451	12.478	1.00	30.64
	ATOM	4536	CD2	LEU :	В	252	11.453	97.937	12.008	1.00	29.71
	ATOM .	4537	С	LEU :	В	252	11.860	95.417	9.396	1.00	29.11
10	ATOM	4538	0	LEU	В	252	11.009	96.245	9.077	1.00	29.16
	ATOM:	4539	N	GLY :	В	253	12.483	94.655	8.506	1.00	30.27
	ATOM	4540	CA	GLY	В	253	12.154	94.786	7.092	1.00	30.40
	MOTĄ	4541	С	GLY	В	253	12.909	95.940	6.447	1.00	31.85
	ATOM	4542	0	GLY	В	253	12.677	96.272	5.291	1.00	31.62
15	MOTA	4543	N	GLN	В	254	13.825	96.545	7.212	1.00	32.10
	MOTA	4544	CA	GLN	В	254	14.653	97.665	6.754	1.00	30.81
	ATOM	4545	CB	GLN	В	254	13.814	98.933	6.559	1.00	31.22
	ATOM	4546	CG	GLN	В	254	13.195	99.477	7.836	1.00	31.70
	MOTA	4547	CD	GLN	В	254	12.307	100.677	7.595	1.00	30.46
20	MOTA	4548	OE1	GLN	В	254	12.766	101.814	7.605	1.00	33.00
	MOTA	4549	NE2	GLN	В	254	11.023	100.432	7382	1.00	32.32
	ATOM	4550	С	GLN	В	254	15.777	97.915	7.759	1.00	30.56
	MOTA	4551	0	GLN	В	254	15.697	97.455	8.905	1.00	30.99
	MOTA	4552	N	PRO	В	255	16.849	98.631	7.351	1.00	28.81
25	MOTA	4553	CD	PRO	В	255 .	17.047	99.200	6.003	1.00	29.65
	MOTA	4554	CA	PRO	В	255	17.990	98.918	8.228	1.00	26.75
	MOTA	4555	CB	PRO	В	255	18.932	99.751	7.346	1.00	28.90
	ATOM	4556	CG	PRO	В	255	18.535	99.399	5.948	1.00	28.37
	ATOM	4557	С	PRO	В	255	17.565	99.701	9.461	1.00	25.44
30	ATOM	4558	0	PRO	В	255	16.855	100.696	9.371	1.00	23.84
	MOTA	4559	N	ILE	В	256	17.998	99.221	10.617	1.00	25.79
	MOTA	4560	CA	ILE	В	256	17.662	99.842	11.893	1.00	22.03
	MOTA	4561	CB	ILE	В	256	18.048	98.931	13.089	1.00	20.49
	MOTA	4562	CG2	LLE	В	256	19.519	98.531	13.046	1.00	16.83
35	MOTA	45,63	CG1	ILE	B	256	17.676	99.562	14.444	1.00	22.30

	ATOM	4564	CD1	ILE	В	256	16.380	100.346	14.446	1.00	22.57
	ATOM	4565	С	ILE	В	256	18.218	101.261	12.029	1.00	20.33
	MOTA	4566	0	ILE	В	256	17.506	102.163	12.473	1.00	23.40
	ATOM	4567	N	PHE	В	257	19.472	101.468	11.641	1.00	20.97
5	MOTA	4568	CA	PHE	В	257	20.091	102.794	11.734	1.00	21.60
	MOTA	4569	CB	PHE	В	257	21.223	102.800	12.777	1.00	21.88
	MOTA	4570	CG	PHE	В	257	20.968	101.972	14.019	1.00	20.01
	MOTA	4571	CD1	PHE	В	257	19.896	102.256	14.857	1.00	20.95
	MOTA	4572	CD2	PHE	В	257	21.811	100.924	14.350	1.00	19.46
10	MOTA	4573	CE1	PHE	В	257 ,	19.677	101.507	16.001	1.00	21.15
	ATOM	4574	CE2	PHE	В	257	21.595	100.170	15.494	1.00	20.25
	MOTA	4575	CZ	PHE	В	257	20.527	100.461	16.319.	1.00	17.61
•	ATOM	4576	С	PHE	B	257	20.625	103.303	10.378	1.00	23.72
	MOTA	4577	0	PHE	В	257	21.799	103.116	10.050	1.00	24.92
15	MOTA	4578	N	PRO	В	258	19.774	103.959	9.571	1.00	24.77
	MOTA	4579	CD	PRO	В	258	18.355	104.232	9.859	1.00	24.97
	MOTA	4580	CA .	PRO	В	258	20.173	104.492	8.258	1.00	26.83
	MOTA	4581	CB	PRO	В	258	18.838	104.562	7.526	1.00	25.37
	ATOM	4582	CG	PRO	В	258	17.861	104.907	8.601	1.00	26.59
20	ATOM	4583	С	PRO	В	258	20.801	105.892	8.333	1.00	27.49
	ATOM	4584	0	PRO	В	258	20.148	106.890	8.027	1.00	29.44
	ATOM	4585	N	GLY	B	259	22.072	105.958	8.723	1.00	28.58
	MOTA	4586	CA	GLY	B	259	22.763	107.238	8.809	1.00	30.88
	MOTA	4587	C·	GLY	В	259	23.066	107.815	7.430	1.00	32.75
25	ATOM	4588	0	GLY	В	259	23.074	107.080	6.441	1.00	32.73
	ATOM	4589	N	ASP	В	260	23.304	109.127	7.353	1.00	33.18
	ATOM	4590	CA	ASP	В	260	23.580	109.762	6.066	1.00	34.42
	MOTA	4591	CB	ASP	В	260	22.530	110.847	5.730	1.00	35.56
	ATOM.	4592	CG	ASP	В	260	22.547	112.072	6.649	1.00	37.21
30	ATOM	4593	OD1	ASP	В	260	21.477	112.692	6.836	1.00	38.35
	MOTA	4594	OD2	ASP	В	260	23.622	112.424	7.172	1.00	41.05
	MOTA	4595	С	ASP	В	260	25.004	110.298	5.897	1.00	34.80
	ATOM	4596	0	ASP	В	260	25.282	110.976	4.901	1.00	35.69
	MOTA	4597	N	SER	В	261	25.919	110.032	6.843	1.00	34.20
35	ATOM	4598	CA	SER	В	261	27.262	110.591	6.653	1.00	33.70

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	MOTA	4599	CB	SER	В	261		27.282	112.065	7.073	1.00	34.65
	MOTA	4600	OG	SER	В	261		26.660	112.247	8.333	1.00	34.15
	MOTA	4601	C	SER	В	261		28.405	109.854	7.338	1.00	33.14
	ATOM	4602	0 -	SER	В	261		29.513	109.776	6.792	1.00	35.18
5	ATOM	4603	N	GLY	B	262		28.169	109.389	8.546°	1.00	31.51
	MOTA	4604	CA	GLY.	В	262		29.215	108.741	9.316	1.00	28.23
	MOTA	4605	С	GLY	В	262		29.127	109.228	10.749	1.00	29.20
	MOTA	4606	0	GLY	В	262		29.340	108.475	11.699	1.00	27.66
•	ATOM	4607	N	VAL	В	263		28.734	110.491	10.879	1.00	28.32
10	ATOM	4608	CA	VAL	В	263		28.510	111.127	12.161	1.00	27.43
	MOTA	4609	СВ	VAL	В	263 ·		28.983	112.591	12,157	1.00	27.60
	MOTA	4610	CG1	VAL	В	263		28.678	113.246	13.498	1.00	28.91
	ATOM	4611	CG2	VAL	В	263		30.474	112.661	11.844	1.00	26.99
	ATOM	4612	С	VAL	В	263		27.012	111.072	12.434	1.00	27.34
15	ATOM	4613	0	VAL	В	263		26.580	110.866	13.567	1.00	27.77
	MOTA	4614	N	ASP	В	264		26.226	111.198	11.351	1.00	24.33
	MOTA	4615	CA	ASP.	В	264		24.772	111.100	11.420	1.00	22.03
	MOTA	4616	СВ	ASP	·B	264		24.145	111.447	10.064	1.00	22.91
	ATOM	4617	CG	ASP	В	264		22.630	111.375	10.086	1.00	23.28
.20	MOTA	4618	OD1	ASP	В	264	•	22.010	112.133	10.859	1.00	27.20
	ATOM	4619	OD2	ASP	В	264		22.062	110.557	9.339	1.00	28.80
	ATOM	4620	С	ASP	В	264		24.384	109.673	11.814	1.00	20.79
	MOTA	4621	0	ASP	В	264		23.292	109.420	12.307	1.00	22.24
•	ATOM	4622	И .	GLN	В	265	•	25.305	108.749	11.607	1.00	19.00
25	ATOM	4623	CA	GLN	В	265	•	25.086	107.361	11.963	1.00	20.26
	MOTA	4624	CB	GLN	В	265		26.275	106.513	11.496	1.00	16.83
	MOTA	4625	CG	GLN	В	265		26.099	105.018	11.692	1.00	22.64
	MOTA	4626	CD	GLN	В	265		24.868	104.484	10.994	1.00	24.93
	ATOM	4627	OE1	GLN	В	265		24.425	105.033	9.974	1.00	27,28
30	ATOM	4628	NE2	GLN	В	265		24.308	103.408	11.538	1.00	26.87
	ATOM	4629	С	GLN	В	265		24.892	107.241	13.493	1.00	20.32
	MOTA	4630	0	GLN	В	265		24.091	106.433	13.951	1.00	19.37
	ATOM	4631	N	TEU	В	266		25.612	108.079	14.275	1.00	22.23
	ATOM	4632	CA	ĹEU	В	266		25.469	108.062	15.742	1.00	24.94
35	ATOM	4633	CB	LEU	В	266		26.575	108.844	16.472	1.00	22.54

	MOTA	4634	CG	LEU H	3	266	,	26.592	108.702	18.020	1.00	22.64
	ATOM	4635	CD1	LEU I	3	266	4	26.751	107.248	18.440	1.00	18.03
	MOTA	4636	CD2	LEU I	3	266	:	27.695	109.542	18.637	1.00	19.32
	MOTA	4637	С	LEU I	3	266		24.099	108.589	16.134	1.00	25.37
5	ATOM	4638	0	LEU I	В	266		23.478	108.074	17.064	1.00	28.29
	ATOM	4639	N	VAL !	В	267		23.625	109.599	15.391	1.00	24.88
	ATOM	4640	CA.	VAL I	В	267		22.312	110.198	15.622	1.00	24.12
	ATOM	4641	СВ	VAL :	В	267		22.065	111.430	14.716	1.00	24.95
	ATOM	4642	CG1	VAL	В	267		20.651	111.967	14.901	1.00	23.98
10	ATOM	4643	CG2	VAL	B	267		23.083	112.522	15.004	1.00	25.79
	MOTA	4644	С	VAL	В	267		21.183	109.182	15.424	1.00	24.25
	MOTA	4645		VAL	В	267		20.201	109.176	16.177	1.00	23.82
-	ATOM	4646	N	GLU	В	268		21.319	108.324	14.408	1.00	25.05
	ATOM	4647	CA	GLU	В	268		20.299	107.307	14.122	1.00	23.51
15	ATOM	4648	CB	GLU	В	268		20.515	106.693	12.732	1.00	24.47
	ATOM	4649	CG	GLU	В	268		20.293	107.676	11.584	1.00	21.75
	MOTA	4650	CD	GLU	В	268		18.934	108.349	11.638	1.00	18.57
	MOTA	4651	OE1	GLU	В	268		18.881	109.594	11.611	1.00	22.02
	MOTA	4652	OE2	GLU	В	268		17.923	107.632	11.706	1.00	23.39
20	ATOM	4653	С	GLU	В	268		20.292	106.224	15.207	1.00	23.03
	ATOM	4654	0	GLU	В	268		19.237	105.731	15.613	1.00	22.81
	MOTA	4655	N	ILE	В	269		21.472	105.884	15.689	1.00	21.74
	ATOM	4656	CA	ILE	В	269	•	21.612	104.898	16.744	1.00	24.46
	MOTA	4657	CB	ILE	В	269		23.102	2 104.574	16.970	1.00	23.40
25	ATOM	4658	CG2	Į ILE	В	269		23.314	1 103.814	18.275	1.00	22.87
	ATOM	4659	CG:	l ILE	B	269		23.656	5 103.780	15.776	1.00	20.00
	MOTA	4660	CD:	1 ILE	E	269		25.16	103.648	15.773	1.00	14.35
	MOTA	4661	С	ILE	E	3 269		20.998	3 105.450	18.041		26.26
	MOTA	4662	0	ILE	E	3 269		20.16	6 104.797	18.672		26.78
30	ATOM	4663	N	ILE	E	3 270		21.40	6 106.677	18.404		27.54
	MOTA	4664	CA	ILE	E	3 270		20.91	1 107.364	19.600		29.63
	ATOM	4665	CB	ILE	ŀ	B 270			4 108.780			27.82
	ATOM	4666	CG	2 ILE	: 1	В 270		20.56	1 109.740	20.414		0 27.92
	MOTA	4667	CG	1. ILE		в 270		22.85	9 108.71	20.483		0 24.59
35	MOTA	4668	CE	1 ILE		B 270		23.78	4 109.873	3 20.192	1.0	0 20.57

•	ATOM	4669	C	ILE	В	270	19.380	107.439	19.625	1.00	31.35
	MOTA	4670	0	ILE	B	270	18.766	107.336	20.688	1.00	31.68
	MOTA	4671	N	LYS	В	271	18.762	107.605	18.456	1.00	31.75
	ATOM	4672	CA	LYS	В	271	17.298	107.675	18.368	1.00	31.08
5	ATOM	4673	CB	LYS	В	271	16.859	107.825	16.907	1.00	32.98
	ATOM	4674	CG	LYS	В	271	16.767	109.266	16.432	1.00	35.15
	ATOM	4675.	CD	LYS	В	271	15.829	109.383	15.237	1.00	39.78
	ATOM	4676	CE	LYS	В	271	16.337	110.374	14.199	1.00	40.13
	ATOM	4677	NZ	LYS	В	271	15.626	110.220	12.895	1.00	43.28
10	ATOM	4678	C .	LYS	В	271	16.635	106.430	18.973	1.00	31.09
	ATOM	4679	0	LYS	В	271	15.500	106.495	19.450	1.00	31.32
	MOTA	4680	И	VAL	В	.272	17.341	105.297	18.936	1.00	30.13
	ATOM	4681	ĊA	VAL	В	272	16.820	104.033	19.463	1.00	29.49
	ATOM	4682.	СВ	VAL	В	272	17.077	102.865	18.479	1.00	29.16
15	ATOM	4683	CG1	VAL	В	272	16.785	101.520	19.139	1.00	26.10
	MOTA	4684	CG2	VAL	В	272	16.254	103.037	17.208	1.00	28.45
	ATOM	4685	С	VAL	В	272	17.439	103.673	20.811	1.00	29.05
	ATOM	4686	0	VAL	В	272	16.729	103.343	21.753	1.00	30.91
	ATOM	4687	N	LEU	В	273	18.763	103.706	20.885	1.00	29.13
20	ATOM	4688	CA	LEU	B.	273	19.475	103.352	22.106	1.00	28.98
	MOTA	4689	CB	LEU	В	273	20.936	103.024	21.786	1.00	27.13
	ATOM	4690	CG	LEU	В	273 ,	21.202	101.678	21.103	1.00	25.76
-	ATOM	4691	CD1	LEU	В	273	22.652	101.264	21.268	1.00	24.23
	MOTA	4692	CD2	LEU	В	273	20.273	100.605	21.641	1.00	27.25
25	MOTA	4693	С	LEU	В	273	19.413	104.463	23.156	1.00	31.27
	MOTA	4694	0	LEU	В	273	19.689	104.233	24.344	1.00	33.10
	ATOM	4695	N	GLY	В	274	19.081	105.664	22.709	1.00	30.29
•	MOTA	4696	CA	GLY	В	274	19.030	106.793	23.599	1.00	28.69
	ATOM	. 4697	С	GLY	В	274	20.424	107.311	23.816	1.00	28.22
30	ATOM	4698	· O	GLY	В	274	21.393	106.622	23.494	1.00	27.85
	ATOM	4699	N	THR	В	275	20.548	108.513	24.353	1.00	28.54
	ATOM	4700	CA	THR	В	275	21.874	109.068	24.585	1.00	29.17
	MOTA	4701	CB	THR	В	275	21.782	110.445	25.229	1.00	28.46
	ATOM	4702	OG1	THR	В	275	20.977	111.305	24.448	1.00	31.45
35	MOTA	4703	CG2	THR	В	275	23.127	111.112	25.418	1.00	27.39

	ATOM	4704	С	THR B 275	22.723 108.132	25.439	1.00 29.25
	MOTA	4705	0	THR B 275	22.255 107.618	26.455	1.00 30.69
	MOTA	4706	N	PRO B 276	23.989 107.893	25.036	1.00 29.38
	MOTA	4707	CD	PRO B 276	24.626 108.455	23.832	1.00 27.67
5	ATOM	4708	CA	PRO B 276	24.897 107.021	25.778	1.00 28.22
	MOTA	4709	СВ	PRO B 276	26.006 106.733	24.770	1.00 27.80
	ATOM	4710	CG	PRO B 276	26.039 107.941	23.901	1.00 24.60
	MOTA	4711	С	PRO B 276	25.462 107.752	26.996	1.00 30.33
	MOTA	4712	0	PRO B 276	25.782 108.942	26.918	1.00 28.30
10	MOTA	4713	N	THR B 277	25.564 107.036	28.122	1.00 30.45
	ATOM	4714	CA	THR B 277	26.072 107.619	29.354	1.00 30.41
	ATOM	4715	CB	THR B 277	25.700 106.767	30.576	1.00 29.19
	ATOM	4716	OG1	THR B 277	26.399 105.542	30.593	1.00 29.41
	MOTA	4717	CG2	THR B 277	24.222 106.467	30.690	1.00 28.20
15	MOTA	4718	C	THR B 277	27.571 107.845	29.282	1.00 31.58
	ATOM	4719	0	THR B 277 .	28.264 107.203	28.490	1.00 30.78
	ATOM	4720	N	ARG B 278	28.063 108.773	30.111	1.00 32.07
	ATOM	4721	CA	ARG B 278	29.485 109.104	30.148	1.00 33.38
	ATOM	4722	CB	ARG B 278	29.761 110.140	31.245	1.00 36.19
20	MOTA	4723	CG	ARG B 278	29.811 109.553	32.648	1.00 40.29
	ATOM	4724	CD	ARG B 278	28.417 109.370	33.243	1.00 44.36
	ATOM	4725	NE	ARG B 278	28.111 107.962	33.513	1.00 44.31
	MOTA	4726	CZ	ARG B 278	26.871 107.469	33.607	1.00 46.69
	MOTA	4727	NH	1 ARG B 278	25.808 108.271	33.485	1.00 47.71
25	ATOM	4728	NH:	2 ARG B 278	26.690 106.167	33.831	1.00 46.93
	ATOM	4729	С	ARG B 278	30.340 107.855	30.356	1.00 32.74
	ATOM	4730	0	ARG B 278	31.452 107.760	29.840	1.00 34.25
	ATOM	4731	N	GLU B 279	29.811 106.890	31.101	1.00 32.02
	MOTA	4732	CA	GLU B 279	30.529 105.650	31.348	1.00 31.30
30	ATOM	4733	CB	GLU B 279	29.874 104.848	32.482	
•	ATOM	4734	CG	GLU B 279	30.599 103.550	32.841	1.00 35.58
	MOTA	4735	c c	GLU B 279	32.113 103.698	32.960	1.00 36.93
•	MOTA	4736	o ÓE	E1 GLU B 279	32.825 102.674	32.834	
	ATOM	4737	7 OF	E2 GLU B 279	32.589 104.831	. 33.183	1.00 39.38
35	ATOM	4738	3 C	GLU B 279	30.601 104.817	30.0.68	1.00 28.54

	ATOM	4739	0	GLU	В	279	31.653	104.304	29.722	1.00	29.69
•	ATOM	4740	N	GLN	В	280	29.471	104.709	29.371	1.00	27.39
	ATOM	4741	CA	GLN	В	280 .	29.390	103.959	28.115	1.00	26.77
	MOTA	4742	CB	GLN	В	280	27.947	103.942	27.595	1.00	24.23
5	ATOM	4743 *	CG	GLN	В	280	27.039	102.979	28.355	1.00	21.13
	ATOM	4744	CD	GLN	В	280	25.564	103.172	28.073	1.00	18.64
	ATOM	4745	OE1	GLN	В	280	25.120	104.256	27.712	1.00	21.44
	MOTA	4746	NE2	GLN	В	280	24.789	102.109	28.242	1.00	22.07
	MOTA	4747	С	GLŅ	В	280	30.356	104.535	27.077	1.00	27.30
10	MOTA	4748	0	GLN	В	280	31.039	103.787	26.372	1.00	28.93
	MOTA	4749	N	ILE	В	281	30.441	105.868	27.023	1.00	28.72
	MOTA	4750	CA	ILE	В	281	31.350	106.555	26.106	1.00	28.63
	ATOM	4751	CB	ILE	В	281	31.120	108.079	26.100	1.00	29.61
	MOTA	4752	CG2	ILE	В	281	32.235	108.798	25.344	1.00	30.25
15	ATOM	4753	CG1	ILE	В	281	29.758	108.407	25.489	1.00	28.88
	ATOM	4754	CD1	ILE	В	281	29.439	109.885	25.460	1.00	28.04
	ATOM	4755	С	ILE	В	281	32.809	106.261	26.445	1.00	30.30
	ATOM	4756	0	ILE	B	281	33.652	106.142	25.549	1.00	30.65
	ATOM	4757	N	ARG	В	282	33.109	106.138	27.739	1.00	30.28
20	ATOM	4758	CA	ARG	В	282	34.470	105.848	28.181	1.00	29.89
	ATOM	4759	CB	ARG	В	282	34.605	106.070	29.700	1.00	33.28
•	MOTA	4760	CG	ARG	B	282	35.923	106.718	30.111	1.00	35.52
•	MOTA	4761	CD	ARG	В	282	35.700	107.947	30.990	1.00	40.01
	MOTA	4762	NE	ARG	В	282	36.769	108.944	30.842	1.00	41.68
25	MOTA	4763	CZ	ARG	В	282	38.015	108.791	31.316	1.00	44.99
	ATOM	4764	NH1	ARG	В	282	38.374	107.669	31.946	1.00	45.52
	ATOM	4765	NH2	ARG	В	282	38.911	109.763	31.150	1.00	46.24
	MOTA	4766	С	ARG	В	282	34.855	104.413	27.816	1.00	28.46
	ATOM	4767	0	ARG	В	282	36.016	104.111	27.549	1.00	28.25
30	ATOM	4768	N	GLU	В	283	33.869	103.536	27.794	1.00	28.29
	ATOM	4769	CA	GLU	В	283	34.099	102.143	27.448	1.00	30.36
	MOTA	4770	CB	GLÜ	В	283	32.931	101.276	27.929	1.00	30.84
٠	ATOM	4771	CG	GLU	В	283	32.371	101.707	29.277	1.00	34.73
	ATOM	4772	CD	GLU	В	283	31:757	100.572	30.063	1.00	35.22
35	ATOM	4773	OE1	GLU	В	283	30.531	100.604	30.287	1.00	35.59

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	MOTA	4774	OE2	GLU B	283	32.505	99.654	30.460	1.00 3	
	ATOM	4775	C	GLU B	283	34.314	101.983	25.938	1.00 3	
	MOTA	4776	0 (GLU B	283	35.030	101.083	25.494	1.00	•
	ATOM	4777	N I	MET B	284	33.696	102.869 .	25.153	1.00	31.90
5	MOTA	4778	CA	MET B	284	33.824	102.828	23.694	1.00	33.07
	ATOM	4779	CB	MET B	284	32.766	103.709	23.010	1.00	31.27
	MOTA	4780	CG	MET B	284	31.336	103.320	23.397	1.00	28.45
•	MOTA	4781	SD	MET B	284	30.074	103.769	22.183	1.00	28.71
	MOTA	4782	CE	MET B	284	29.055	104.901	23.120	1.00	28.37
10	ATOM	4783	С	MET B	284	35.274	103.066	23.209	1.00	35.36
	MOTA	4784	0	MET B	284	35.627	102.713	22.095	1.00	36.19
	ATOM .	4785	N	ASN B	285	36.126	103.628	24.096	1.00	40.09
	ATOM	4786	CA	ASN B	285	37.565	103.878	23.885	1.00	41.52
	ATOM	4787	СВ	ASN B	285	38.228	102.601	23.372	1.00	41.35
15	MOTA	4788	CG	ASN B	285	39.010	101.810	24.425	1.00	41.10
	MOTA	4789	OD1	ASN B	285 ·	38.641	100.687	24.743	1.00	39.10
	MOTA	4790	ND2	ASN B	285	40.070	102.412	24.949	1.00	39.99
	MOTA	4791	С	ASN B	285	37.889	105.060	22.969	1.00	43.22
	ATOM	4792	0	ASN B	285	38.927	105.089	22.316	1.00	44.35
20	ATOM	4793	N	PRO B	286	36.949	106.038	22.916	1.00	42.77
	ATOM	4794	CD	PRO B	286	35.613	105.535	22.609	1.00	.42.20
	MOTA	4795	CA	PRO B	286	37.137	107.295	22.114	1.00	43.36
	ATOM	4796	СВ	PRO B	286	35.773	3 107.946	22.211	1.00	42.17
	ATOM	4797	CG	PRO B	286	34.880	106.742	22.145	.1.00	41.91
25	ATOM	4798	С	PRO B	3 286	38.281	108.205	22.503	1.00	45.30
	ATOM	4799	0	PRO E	3 286	39.043	3 108.744	21.711	1.00	46.02
	ATOM	4800	N	ASN E	3 287	38.364	108.297	23.816	1.00	46.61
	MOTA	4801	CA	ASN E	3 287	39.252	2 109.173	24.502	1.00	46.03
	MOTA	4802	СВ	ASN E	3 287	40.69	5 109.000	24.024	1.00	46.35
30	MOTA	4803	CG	ASN E	3 287	41.48	3 108.033	24.931	1.00	47.41
	MOTA	4804	. 001	L ASN I	в 287	42.70	2 108.016	24.913	1.00	47.27
	MOTA	4805	5 ND2	2 ASN 1	в 287	40.76	9 107.244	25.730	1.00	48.69
	MOTA	4806	5 C	ASN :	в 287	38.57	2 110.544	24.324	1.00	45.96
	ATOM	480	7 0	ASN	в 287	37.33	8 110.570	24.291	1.00	46.40
35	MOTA	4808	3 и	TYR	В 288	39.23	4 111.651	24.213	1.00	45.99
									•	

	ATOM	4809	CA	TYR	В	288	38.481	112.942	24.243	1.00	47.00
	MOTA	4810	СВ	TYR	В	288 .	39.422	114.014	23.729	1.00	46.88
	ATOM	4811	CG	TYR	В	288	39.402	114.302	22.265	1.00	47.95
	ATOM	4812	CD1	TYR	В	288	39.909	113.377	21.352	1.00	48.31
.5	ATOM	4813	CE1	TYR	В	288	39.914	113.642	19.993	1.00	47.74
	ATOM	4814	CD2	TYR	В	288	38.901	115.503	21.768	1.00	47.29
	MOTA	4815	CE2	TYR	В	288	38.902	115.775	20.411	1.00	47.45
	ATOM	4816	CZ	TYR	В	288	39.410	114.841	19.528	1.00	48.12
	ATOM	4817	ОН	TYR	В	288	39.414	115.108	18.176	1.00	48.51
10	ATOM .	4818	С	TYR	В	288.	37.066	113.054	23.631	1.00	48.12
	ATOM	4819	0	TYR	В	288	36.086	112.693	24.291	1.00	48.23
	ATOM	4820	N	THR	В	289	36.934	113.523	22.398	1.00	49.01
	ATOM	4821	CA	THR	В	289	35.644	113.609	21.677	1.00	50.53
	ATOM	4822	CB	THR	В	289	35.006	112.211	21.583	1.00	49.77
15	ATOM	4823	OG1	THR	В	289	35.396	111.568	20.363	1.00	47.97
	ATOM	4824	CG2	THR	В	289	33.491	112.312	21.629	1.00	48.53
	ATOM	4825	C	THR	B.	289	34.609	114.574	22.268	1.00	52.67
	ATOM	4826	0	THR	В	289	33.934	114.254	23.256	1.00	53.68
	ATOM	4827	N	GLU	В	290	34.502	115.768	21.629	1.00	54.04
20	ATOM	4828	CA	GLU	В	290	33.338	116.686	21.857	1.00	55.39
	ATOM	4829	CB	GLU	В	290	33.580	117.961	21.042	1.00	56.12
	ATOM	4830	CG	GLU	В	290	33.431	119.249	21.842	1.00	57.86
	ATOM	4831	CD	GLU	В	290	34.524	119.422	22.886	1.00	59.39
	ATOM	4832	OE1	GLU	В	290	35.513	120.138	22.604	1.00	59.57
25	ATOM	4833	OE2	GLU	В	290	34.391	118.840	23.987	1.00	60.09
	ATOM	4834	C	GLU	В	290	31.900	116.202	21.684	1.00	56.39
	ATOM	4835	Ο.	GLU	B	290	31.408	116.094	20.558	1.00	55.69
	ATOM	4836	N	PHE	В	291	31.251	115.905	22.809	1.00	57.38
	ATOM	4837	CA	PHE	В	291	29.884	115.385	22.788	1.00	58.23
30	ATOM	4838	CB	PHE	В	291	29.463	114.915	24.213	1.00	58.40
	ATOM	4839	CG	PHE	В	291	30.191	115.516	25.370	1.00	59.05
	ATOM	4840	CD1	PHE	В	291	29.563	116.464	26.167	1.00	59.39
	MOTA	4841	CD2	PHE	В	291	31.500	115.157	25.668	1.00	58.98
	MOTA	4842	CE1	PHE.	В	291	30.226	117.041	27.239	1.00	59.94
35	MOTA	4843	CE2	PHE	В	291	32.168	115.732	26.736	.1.00	59.79

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	MOTA	4844 CZ	PHE B 291	31.530 116.674		1.00 59.54
	ATOM	4845 C	PHE B 291	28.841 116.334	22.206	1.00 59.10
	MOTA	4846 O	PHE B 291	28.725 116.435		1.00 59.54
	ATOM	4847 N	LYS B 292	28.070 117.028	23.074	1.00 59.05
5	MOTA	4848 CA	LYS B 292	26.995 117.952		1.00 59.28
	MOTA	4849 CB	LYS B 292	27.321 118.665	21.317	1.00 60.62
	ATOM	4850 CG	LYS B 292	26.818 117.941	20.064	1.00 60.64
	ATOM	'4851 CD	LYS B 292	25.623 118.652	19.431	1.00 61.74
	ATOM	4852 CE	LYS B 292	24.974 117.805		1.00 61.38
10	ATOM	4853 NZ	LYS B 292	24.644 116.430	18.826	1.00 63.08
	MOTA	4854 C	LYS B 292	25.657 117.203	22.558	1.00 58.54
	MOTA	4855 O	LYS B 292	24.670 117.727	22.031	1.00 59.16
	ATOM	4856 N	PHE B 293	25.645 115.965	23.058	1.00 57.33
	ATOM	4857 CA	PHE B 293	24.461 115.098	23.022	1.00 55.98
15	MOTA	4858 CB	PHE B 293	24.787 113.698	23.560	1.00 54.70
	ATOM	4859 CG	PHE B 293	26.048 113.105	23.001	1.00 53.63
	· ATOM	4860 CD	1 PHE B 293	26.233 112.994	21.631	1.00 53.34
	ATOM	4861 CD	2 PHE B 293	27.054 112.665	23.844	1.00 53.03
	MOTA	4862 CE	1 PHE B 293	27.397 112.455	21.114	1.00 52.99
20	MOTA	4863 CE	2 PHE B 293	28.219 112.123	23.335	1.00 53.14
	ATOM	4864 CZ	PHE B 293	28.393 112.019	21.967	1.00 53.19
	MOTA	4865 C	PHE B 293	23.246 115.676		1.00 54.80
	MOTA	4866 O	PHE B 293	23.260 115.859	24.970	1.00 54.06
	MOTA	4867 N	PRO B 294	22.165 115.944		1.00 54.22
25	MOTA	4868 CI	PRO B 294	22.067 115.735	21.547	1.00 54.04
	ATOM	4869 C	A PRO B 294	20.913 116.473		1.00 53.37
	ATOM:	4870 C	B PRO B 294	20.163 116.990		1.00 54.04
	MOTA	4871 C	G PRO B 294	21.098 116.803	•	1.00 53.92
	ATOM	4872 C	PRO B 294	20.100 115.372		1.00 52.60
30	MOTA	4873 0	PRO B 294	19.065 114.955	_	1.00 53.54
	ATOM	4874 N	GLN B 295	20.595 114.909		
	ATOM	4875 C	CA GLN B 295	19.978 113.84		
	ATOM	4876	CB GLN B 295	19.970 114.22		
	ATOM	4877	CG GLN B 295	21.056 113.53		
35	5 ATOM	4.878	CD GLN B 295	20.835 112.03	7 28.656	1.00 48.49

	ATOM	4879	OE1	GLN B 295	19.740 11	1.523 2	28.414	1.00	49.23	•
	ATOM	4880	NE2	GLN B 295	.21.880 11	1.325	29.067	1.00	47.84	
	ATOM	4881	С	GLN B 295	18.576 11	3.436	25.724	1.00	49.95	
	MOTA	4882	0	GLN B 295	17.598 11	4.139 . 2	25.982	1.00	50.65	
5	ATOM	4883	N .	ILE B 296	18.495 11	2.285	25.044	1.00	49.14	
	ATOM	4884	CA .	ILE B 296	17.226 11	1.755	24.541	1.00	47.84	
	ATOM	4885	СВ	ILE B 296	17.139 11	1.751	22.989	1.00	47.05	
	ATOM	4886	CG2	ILE B 296	18.317 11	2.482	22.362	1.00	46.60	•
	MOTA	4887	CG1	ILE B 296	17.011 11	0.332	22.422	1.00	47.81	
10	ATOM	4888	CD1	ILE B 296	15.633 11	.0.022	21.879	1.00	47.64	
	MOTA	4889	С	ILE B 296	16.928 11	0.370	25.129	1.00	47.17	
•	ATOM	4890	0	ILE B 296	17.835 10	9.662	25.572	1.00	47.85	
<i>,</i>	MOTA	4891	И	LYS B 297	15.650 11	.0.008	25.163	1.00	46.24	
	ATOM	4892	ĊA	LYS B 297	15.228 10	8.737	25.734	1.00	46.31	
15	MOTA	4893	CB	LYS B 297	13.770 10	8.819	26.195	1.00	47.40	
	ATOM	4894	CG	LYS B 297	13.624 10	9.112	27.682	1.00	48.65	
	ATOM	4895	CD	LYS B 297	13.321 11	.0.582	27.938	1.00	49.80	
	MOTA	4896	CE	LYS B 297	13.284 11	.0.905	29.431	1.00	49.46	
	MOTA	4897	NZ	LYS B 297	14.326 11	1.907	29.813	1.00	49.34	
20	MOTA	4898	С	LYS B 297	15.394 10	7.577	24.766	1.00	46.58	
	MOTA	4899	0	LYS B 297	15.210 10	7.717	23.554	1.00	46.65	
	ATOM	4900	N	ALA B 298	15.725 10	6.420	25.322	1.00	45.88	
•	ATOM	4901	ĊA	ALA B 298 .	15.898 10	5.221	24.529	1.00	45.60	
	ATOM	4902	CB	'ALA B 298	16.747 10	04.203	25.271	1.00	45.85	
25	ATOM	4903	C	ALA B 298	14.549 10)4.623	24.178	1.00	45.64	
	ATOM	4904	0	ALA B 298	13.745 10)4.318	25.061	1.00	45.66	
	MOTA	4905	N	HIS B 299	14.313 10	04.446	22.879	1.00	45.97	
	MOTA	4906	CA	HIS B 299	13.073 10	3.860	22.397	1.00	44.58	
	MOTA	4907	CB.	HIS B 299	12.970 10	04.049	20.883	1.00	44.27	
30	MOTA	4908	CG	HIS B 299	11.687 10	03.567	20.292	1.00	44.81	
	MOTA	4909	CD2	HIS B 299	11.433 10	02.545	19.437	1.00	45.61	
•	ATOM	4910	ND1	HIS B 299	10.469 10	04.151	20.559	1.00	44.53	
	ATOM	4911	CE1	HIS B 299	9.518 10	03.511	19.898	1.00	44.42	
	ATOM	4912	NE2	HIS B 299	10.077 10	02.533	19.208	1.00	44.70	
35	ATOM	4913	С	HIS B 299	13.066 10	02.374	22.760	1.00	44.19	

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	ATOM	4914) H	IS B 299	13.877 10	01.599 2	22.245	L.00 44	.88
	ATOM	4915 · 1	N P	RO B 300	12.166 10	01.963	23.677	1.00 43	.75
	ATOM	4916	CD P	RO B 300	11.186 10	02.819	24.353	1.00 42	.82
	ATOM	4917	CA P	RO B 300	12.068 1	00.575	24.136	1.00 42	.83
5	ATOM	4918	CB P	RO B 300	10.711 1	00.515	24.856	1.00 .42	2.70
	ATOM	4919	ÇG P	RO B 300	10.079 1	01.858	24.663	1.00 42	2.34
	ATOM	4920	C F	PRO B 300	12.133	99.563	22.989	1.00 42	2.56
	ATOM	4921	O E	PRO B 300	11.382	99.659	22.011	1.00 42	2.03
	ATOM	4922	r n	RP B 301	13.050	98.602	23.118	1.00 43	1.90
10	MOTA	4923	CA T	TRP B 301	13.253	97.562	22.110	1.00 42	2.83
	ATOM	4924	CB :	TRP B 301	14.209	96.480	22.629	1.00 4	1.84
	ATOM	4925	CG 5	TRP B 301	15.664	96.775	22.382	1.00 3	9.53
	ATOM	4926	CD2	TRP B 301	16.288	97.049	21.119	1.00 3	
	MOTA	4927	CE2	TRP B 301	17.656	97.263	21.366	1.00 3	•
15	ATOM	4928	CE3	TRP B 301	15.820	97.139	19.806	1.00 3	
	ATOM	4929	CD1	TRP B 301	16.660	96.828	23.314	1.00 3	
	ATOM	4930	NE1	TRP B 301	17.858	97.124	22.716	1.00 3	
	ATOM	4931	CZ2	TRP B 301	18.561	97.554	20.347	1.00 3	
•	MOTA	4932	CZ3	TRP B 301	16.718	97.428	18.798	1.00 3	
20	ATOM	4933	CH2	TRP B 301	18.072	97.635	19.073	1.00	
	MOTA	4934	С	TRP B 301	11.929	96.945	21.634	1.00 4	
	ATOM	4935	0	TRP B 301	11.745	96.702	20.439	1.00	
	ATOM	4936	N	THR B 302	11.011	96.704		1.00	
	MOTA	4937	CÄ	THR B 302	9.703	96.124	22.260	1.00	
25	MOTA	4938	CB	THR B 302	8.907	95.844	23.545	1.00	
	MOTA	4939	OG1	THR B 302	7.551	95.537	23.254		45.99
	ATOM	4940	CG2	THR B 302	8.926	96.984	24.545		44.89
	MOTA	4941	С	THR B 302					45.16
	MOTA	4942	0	THR B 302	8.097				45.19
30	ATOM	4943	N	LYS B 30	9.061		•		44.79
	ATOM	4944	CA	LYS B 30				•	44.92
	ATOM	4945	CB	LYS B 30		100.605			46.86
	ATOM	1 4946	G CG	LYS B 30	_	101.044			49.87
	ATOM	1 4947	7 CD	LYS B 30		100.863			51.82
35	MOTA	4948	3 CE	LYS B 30	5.317	7 102.16	5 19.496	1.00	52.70

	ATOM	4949	NZ	LYS	В	303		4.646	101.983	18.168	1.00	52.78
	ATOM	4950	С	LYS	В	303		9.049	99.465	19.198	1.00	43.33
	MOTA	4951	0	LYS	В	303		8.497	100.069	18.276	1.00	42.39
	ATOM	4952	N	VAL	В	304		10.276	98.956	19.094	1.00	41.74
5	MOTA	4953	CA	VAL	B°	304		11.060	99.081	17.868	1.00	41.90
	MOTA	4954	CB	VAL	В	304		12.546	98.714	18.095	1.00	41.47
•	MOTA	4955	CG1	VAL	В	304	•	13.323	98.774	16.785	1.00	42.51
•	ATOM	4956	CG2	VAL	В	304		13.180	99.628	19.136	1.00	40.62
	ATOM	4.957	C·	VAL	В	304		10.490	98.189	16.766	1.00	41.97
10	ATOM	4958	0	VAL	В	304		10.239	98.644	15.651	1.00	42.22
	ATOM	4959	N	ЬĤЕ	В	305		10.300	96.917	17.090	1.00	41.01
	ATOM.	4960	CA	PHE	В	305		9.787	95.947	16.141	1.00	40.52
	ATOM	4961	CB	PHE	В	305		10.460	94.596	16.352·	1.00	37.42
	MOTA	4962	CG	PHE	В	305		11.955	94.683	16.453	1.00	34.99
15	ATOM	4963	CD1	PHE	В	305		12.572	94.848	17.684	1.00	32.56
	ATOM	4964	CD2	PHE	В	305		12.746	94.603	15.317	1.00	32.98
	ATOM	4965	CE1	PHE	В	305		13.945	94.931	17.783	1.00	31.01
	MOTA	4966 ·	CE2	PHE	В	305		14.121	94.685	15.410	1.00	31.65
	ATOM	4967	CZ	PHE	В	305		14.722	94.848	16.646	1.00	32.89
20	ATOM	4968	С	PHE	В	305		8.269	95.812	16.186	1.00	42.03
•	ATOM	4969	0	PHE	В	305		7.626	96.153	17.177	1.00	43.48
	ATOM	4970	N	ARG	В	306		7.712	95.310	15.087	1.00	43.32
	ATOM	4971	CA	ARG	В	306		6.273	95.115	14.952	1.00	44.86
	ATOM	4972	CB	ARG	В	306		5.951	94.552	13.566	1.00	46.33
25	ATOM	4973	CG	ARG	В	306		5.778	95.620	12.493	1.00	50.23
	ATOM	4974	CD	ARG	В	306		5.129	95.056	11.224	1.00	52.92
	ATOM	4975	NE	ARG	В	306		5.371	93.616	11.070	1.00	55.18
	ATOM	4976	.CZ	ARG	В	306		6.529	93.092	10.663	1.00	55.49
	MOTA	4977	NH1	ARG	В	306		7.512	93.883	10.231	1.00	54.95
30	ATOM	4978	NH2	ARG	В	306		6.696	91.771	10.671	1.00	55.57
	MOTA	4979	С	ARG	В	306		5.730	94.165	16.016	1.00	44.89
	ATOM	4980	0	ARG	В	306		6.452	93.317	16.528	1.00	44.17
	MOTA	4981	N	PRO	В	307		4.430	94.285	16.344	1.00	45.67
	MOTA	4982	CD	PRO	В	307		3.491	95.258	15.759	1.00	45.99
35	ATOM	4983	ĊA	PRO	В	307		3.785	93.418	17.331	1.00	46.08

	MOTA	4984	CB	PRO B 307	2.315	93.850	17.290	1.00 46.12
	MOTA	4985	CG	PRO B 307	2.324	95.214	16.699	1.00 45.88
	MOTA	4986	C	PRO B 307	3.895	91.958	16.911	1.00 47.24
	ATOM	4987	0	PRO B 307	3.956	91.655	15.718	1.00 48.31
5	ATOM	4988	N	ARG B 308	3.923	91.065	17.899	1.00 47.16
	MOTA	4989	CA	ARG B 308	4.024	89.621	17.666	1.00 46.75
	MOTA	4990	CB	ARG B 308	3.070	89.157	16.549	1.00 50.04
	ATOM	4991	CG	ARG B 308	1.887	88.340	17.062	1.00 53.29
	MOTA	4.992	CD	ARG B 308	2.099	86.836	16.875	1.00 57.25
10	ATOM	4993	NE	ARG B 308	3.413	86.383	17.356	1.00 59.65
	ATOM	4994	CZ	ARG B 308	4.243	85.576	16.668	1.00 60.80
	ATOM	4995	NH1	ARG B 308	3.924	85.128	15.446	1.00 61.02
	MOTA	4996	NH2	ARG B 308	5.405	85.218	17.208	1.00 60.97
	MOTA	4997	С	ARG B 308	5.463	89.183	17.371	1.00 45.19
15	ATOM	4998	0	ARG B 308	5.743	87.985	17.319	1.00 45.53
	ATOM	4999	N	THR B 309	6.385	90.141	17.222	1.00 42.87
	ATOM	5000	CA	THR B.309	7.788	89.791	16.994	1.00 40.94
	ATOM	5001	СВ	THR B 309	8.664	91.050	16.914	1.00 39.67
	MOTA	5002	OG1	THR B 309	8.368	91.817	15.767	1.00 38.33
20	MOTA	5003	CG2	THR B 309	10.150	90.765	16.911	1.00 37.91
	MOTA	5004	С	THR B 309	8.260	88.920	18.164	1.00 41.33
	ATOM	5005	0	THR B 309	8.044	89.279	19.329	1.00 42.36
	ATOM	5006	Ŋ	PRO B 310	8.890	87.760	17.888	1.00 39.38
	MOTA	5007	ĊD	PRO B 310	9.182	87.232	16.551	1.00 39.12
25	MOTA	5008	CA	PRO B 310	9.362	86.853	18.938	1.00 37.84
	MOTA	5009	CB	PRO B 310	10.309	85.889	18.203	1.00 37.57
	MOTA	5010	CĠ	PRO B 310	10.409	86.397	16.797	1.00 38.47
	MOTA	5011	C	PRO B 310	10.100	87.595	20.057	1.00 35.75
	MOTA	5012	0	PRO B 310	11.048	88.331	19.803	
30	MOTA	5013	N	PRO B 311	9.676	87.405	21.322	
	ATOM	5014	CD	PRO B 311	8.560	86.544	21.737	1.00 34.88
	MOTA	5015	5 CA	PRO B 311	10.315	5. 88.059	22.473	
•	MOTA	5016	6 CE	B PRO B 311	9.520	87.535	23.676	
	MOTA	5017	7 C	PRO B 311	8.225	<u>.</u>	3 23.095	
35	ATOM	5018	8 C	PRO B 311	11.78	6 87.67	3 22.581	1.00 30.46

•	MOTA	5019	0	PRO 1	В	311	12.619	88.486	22.972	1.00	31.06
	MOTA	5020	N	GLU I	В	312	12.099	86.436	22.198	1.00	29.66
	MOTA	5021	CA	GLU :	В	312	13.475	85.934	22.217	1.00	29.89
	MOTA	5022	CB	GLU :	В	312	13.505	84.444	21.857	1.00	33.20 ⁻
5	MOTA	5023	CG	GLU :	В	312	12.895	83.526	22.907	1.00	37.51
	MOTA	5024	CD	GLU	В	312	11.375	83.517	22.899	1.00	40.54
	ATOM	5025	OE1	GLU :	В	312	10.787	82.991	23.871	1.00	42.54
	ATOM	5026	OE2	GLU	В	312	10.767	84.030	21.926	1.00	42.20
	ATOM	5027	C .	GLU :	В	312	14.360	86.729	21.249	1.00	27.38
10	MOTA	5028	0	GLU	B	312	15.516	87.016	21.549	1.00	27.56
	ATOM	5029	N	ALA	В	313	13.795	87.094	20.093	1.00	26.37
	ATOM.	5030	CA	ALA	В	313	14.522	87.871	19.081	1.00	26.28
	ATOM	5031	CB	ALA	B	313	13.734	87.919	17.773	1.00	25.20
	ATOM	5032	С	ALA	B	313	14.813	89.281	19.593	1.00	24.09
15	ATOM	5033	0	ALA	В	313	15.907	89.804	19.407	1.00	26.54
	ATOM .	5034	N	ILE	В	314	13.834	89.868	20.264	1.00	23.59
	ATOM	5035	CA	ILE	В	314	13.969	91.196	20.846	1.00	23.45
	ATOM	5036	CB	ILE	В	314	12.623	91.678	21.407	1.00	23.44
	ATOM	5037	CG2	ILE	В	314	12.786	92.990	22.165	1.00	26.62
20	MOTA	5038	CG1	ILE	В	314	11.615	91.830	20.262	1.00	24.35
	ATOM	5039	CD1	ILE	В	314	10.334	92.547	20.635	1.00	21.48
	ATOM	5040	С	ILE	В	314	15.029	91.197	21.946	1.00	24.53
•	MOTA	5041	0	ILE	В	3:14	15.885	92.090	22.001	1.00	26.34
	ATOM	5042	N	ALA	В	315	14.987	90.172	22.812	1.00	25.59
25	ATOM	5043	CA	ALA	В	315	15.958	90.036	23.902	1.00	23.39
	ATOM	5044	CB	ALA	В	315	15.575	88.884	24.837	1.00	21.46
	ATOM	5045	С	ALA	В	315	17.370	89.850	23.358	1.00	22.54
	ATOM	5046	0	ALA	В	315	18.298	90.543	23.789	1.00	23.20
	MOTA	5047	N	LEU	В	316	17.537	88.928	22.392	1.00	19.48
30	MOTA	5048	CA	LEU	B	316	18.860	88.708	21.788	1.00	19.69
	MOTA	5049	CB	LEU	В	316	18.826	87.569	20.743	1.00	20.12
•	ATOM	5050	CG	LEU	В	316	20.087	87.365	19.872	1.00	18.08
	ATOM	5051	CD1	LEU	В	316	21.336	87.216	20.716	1.00	13.38
	ATOM	5052	CD2	LEU	В	316	19.926	86.150	18.961	1.00	18.18
35	ATOM	5053	С	LEU	В	316	19.381	90.001	21.155	1.00	17.97

	MOTA	5054	0 3	LEU B	316	20.558	90.325	21.261	1.00 2	0.62
	ATOM	5055	N (CYS B	317	18.492	90.735	20.505	1.00 1	9.40
٠.	ATOM	5056	CA	CYS B	317	18.851	91.990	19.856	1.00 2	2.68
	MOTA	5057	СВ	CYS B	317	17.699	92.511	19.011	1.00 2	4.28
5	MOTA	5058	SG	CYS B	317	18.179	93.846	17.899	1.00 3	6.41
	ATOM	5059	C.	CYS B	317	19.335	93.050	20.850	1.00 2	3.21
	ATOM	5060	0	CYS B	317	20.324	93.751	20.578	1.00 2	1.64
	ATOM	5061	N	SER B	318	18.660	93.157	22.024	1.00 2	3.27
	ATOM	5062	CA	SER B	318	19.084	94.128	23.054	1.00 2	21.97
10	ATOM	5063	CB	SER B	318	18.075	94.219	24.224	1.00 2	23.01
	MOTA	5064	OG	SER B	318	18.004	93.001	24.970	1.00 2	20.21
	MOTA	5065	c ·	SER B	318	20.468	93.765	23.580	1.00 2	21.85
	MOTA	5066	0	SER B	318	21.228	94.637	23.994	1.00 2	22.20
•	MOTA	5067	N	ARG B	319	20.787	92.463	23.558	1.00	21.62
15	MOTA	5068	CA	ARG B	319	22.079	91.969	24.038	1.00	
	ATOM	5069	СВ	ARG B	319	21.937	90.550	24.589	1.00	
	MOTA	5070	CG	ARG E	319	20.671	90.338	25.426	1.00	
	MOTA	5071	CD	ARG E	3 319	20.836	90.757	26.888	1.00	
	MOTA	5072	NE	ARG E	3 319	22.048	91.537	27.127	1.00	
20	MOTA	5073	CZ	ARG H	3 319	23.185	91.038	27.632		27.95
	MOTA	5074	NHl	ARG I	319	23.258	89.769	28.023		26.91
	MOTA	5075	NH2	ARG I	В 319 .	24.256	91.824	27.752		30.55
	MOTA	5076	C	ARG :	B 319	23.167	91.990	22.969		22.03
	MOTA	5077	0	ARG	в 319	24.264	91.471	20120		22.19
25	MOTA	5078	N	LEU	В 320	22.883	92.597			22.15
	MOTA	5079	CA	LEU	B 320	23.883			Α.	18.94
	ATOM	5080	СВ	LEU	в 320	23.382	91.989			17.86
	MOTA	5081	CG	LEU	в 320	23.205	90.487			16.03
	ATOM	5082	CD	1 LEU	В 320	22.562	89.959			17.54
30	ATOM	5083	CD	2 LEU	В 320	24.538	•			16.79
	ATOM	5084	C	LEU	B 320	24.218	3 94.096			16.70
	ATOM	5085	5 0	TEU	в 320	25.36	6 94.449			20.20
	ATOM	5086	5 N	LEU	B 321	23.20	2 94.91			17.99
	ATOM	508	7 CF	Y TEA	B 321	23.39	3 96.31			18.47
35	5 ATOM	508	8 CF	B FEA	В 321	22.23	8 96.82	5 19.19	5 1.00	17.40

	MOTA	5089	CG	LEU	B	321	21.995	96.035	17.906	1.00	17.58
	ATOM	5090	CD1	LEU	В	321	20.591	96.270	17.404	1.00	16.19
	MOTA	5091	CD2	LEU	В	321	23.027	96.403	16.851	1.00	14.68
	ATOM	5092	С	LEU	В	321	23.521	97.113	21.360	1.00	19.25
5	ATOM	5093	0	LEU	В	321	22.659	97.903	21.707	1.00	16.25
	ATOM	5094	N	GLU	В	322	24.612	96.866	22.072	1.00	22.51
	ATOM	5095	CA	GLU	В	322	24.893	97.511	23.354	1.00	23.76
	ATOM	5096	CB	GLU	В	322	25.302	96.425	24.370	1.00	24.61
·	ATOM	5097	CG	GLU	В	322	25.028	96.766	25.829	1.00	30.02
10	MOŢA	5098	CD	GLU	В	322	23.710	96.206	26.325	1.00	27.86
	ATOM	5099	OE1	GLU	В	3,22	23.597	94.974	26.433	1.00	30.28
•	ATOM	5100	OE2	GLU	В	322	22.792	97.003	26.597	1.00	29.21
	ATOM	5101	C	GLU	В	322	26.034	98.493	23.203	1.00	21.13
	ATOM	5102	0	GLU	В	322	27.068	98.149	22.657	1.00	25.15
15	ATOM	5103	N	TYR	В	323	25.859	99.705	23.710	1.00	20.92
	MOTA	5104	CA	TYR	В	323	26.915	100.715	23.636	1.00	21.89
	MOTA	5105	CB	TYR	В	323	26.536	101.953	24.426	1.00	21.76
	MOTA	5106	CG	TYR	В	323	25.653	102.895	23.676	1.00	23.58
	MOTA	5107	CD1	TYR	В	323	26.065	103.451	22.471	1.00	22.37
20	MOTA	5108	CE1	TYR	В	323	25.255	104.328	21.786	1.00	22.17
	MOTA	5109	CD2	TYR	В	323	24.411	103.236	24.174	1.00	23.51
	ATOM	5110	CE2	TYR	В	323	23.595	104.109	23.495	1.00	25.70
	MOTA	5111	CZ	TYR	В	323 ·	24.022	104.653	22.302	1:00	24.73
	ATOM	5112	ОН	TYR	В	323	23.205	105.525	21.625	1.00	24.89
25	MOTA	5113	C	TYR	В	323	28.241	100.186	24.149	1.00	22.26
	MOTA	5114	0	TYR	В	323	29.276	100.338	23.495	1.00	24.24
	ATOM	5115	N	THR	В	324	28.220	99.572	25.333	1.00	21.86
	ATOM	5116	CA	THR	В	324	29.443	99.038	25.915	1.00	19.75
	. ATOM	5117	CB	THR	В	324	29.270	98.807	27.419	1.00	19.32
30	MOTA	5118	OG1	THR	В	324	28.860	100.009	28.035	1.00	18.31
	ATOM	5119	CG2	THR	В	324	30.531	98.334	28.113	1.00	15.93
	ATOM	5120	C	THR	. В	324	29.839	97.776	25.192	1.00	19.46
	ATOM	5121	0	THR	. B	324	29.105	96.794	25.215	1.00	22.97
	MOTA	5122	N	PRC	E	325	30.974	97.805	24.472	1.00	20.22
35	ATOM	5123	CD	PRO	E	3 325	31.870	98.973	24.316	1.00	18.06

	ATOM	5124	CA	PRO B 3	25	31.428	96.663	23.665	1.00 18	3.58
	ATOM	5125	СВ	PRO B 3	25 .	32.754	97.137	23.061	1.00 15	5.36
	ATOM	5126	CG	PRO B 3	25	32.652	98.627	23.073	1.00 1	5.96
	MOTA	5127	С	PRO B 3	125	31.586	.95.364 .	24.452	1.00 2	0.01
5	MOTA	5128	0	PRO B 3	325 .	31.262	94.280	23.936	1.00 1	7.38
	ATOM	5129	N	THR B 3	326	32.077	95.462	25.700	1.00 1	9.19
	ATOM	5130	CA	THR B 3	326	32.259	94.262	26.534	1.00 1	8.37
	ATOM ·	5131	СВ	THR B 3	326	33.212	94.528	27.711	1.00 1	8.49
	MOTA	5132	OG1	THR B	326	32.854	95.724	28.385	1.00 1	9.48
10	ATOM	5133	CG2	THR B	326	34.672	94.623	27.313	1.00 1	.4.73
	ATOM	5134	С	THR B	326	30.925	93.700	27.035	1.00 1	6.62
	ATOM	5135	0	THR B	326	30.866	92.560	27.489	1.00 2	20.08
	MOTA	5136	N	ALA B	327	29.860	94.502	26.935	1.00 1	17.88
	MOTA	5137	CA	ALA B	327	28.508	94.108	27.366	1.00	L7.42
15	ATOM	5138	CB	ALA B	327	27.679	95.344	27.649	1.00	18.02
	ATOM	5139	С	ALA B	327	27.774	93.225	26.342	1.00	18.63
	MOTA	5140	0	ALA B	327	26.790	92.543	26.683	1.00	17.38
	ATOM	5141	N	ARG B	328	28.233	93.249	25.082	1.00	19.14
	. ATOM .	5142	CA	ARG B	328 ,	27.602	92.458	24.016	1.00	15.59
20	ATOM	5143	CB	ARG B	328	28.110	92.919	22.633	1.00	17.66
	MOTA	5144	CG	ARG B	328	27.776	94.355	22.308	1.00	15.25
٠	MOTA	5145	CD	ARG B	328	28.704	94.916	21.237	1.00	18.95
	ATOM	5146	NE	ARG B	328	28.488	96.349	21.048	1:00	19.03
	ATOM	5147	CZ	ARG B	328	29.428	97.187	20.660	1.00	14.77
25	ATOM	5148	ИН	1 ARG B	328	30.594	96.726	20.266	1.00	14.20
	MOTA	5149	NH	2 ARG B	328	29.191	98.491	20.648	1.00	14.60
	ATOM	5150	C	ARG B	328	27.910	90.982	24.169	1.00	11.42
	ATOM	5151	. 0	ARG B	328	29.028	90.61	24.489		11.88
	ATOM	5152	2 N	LEU E	3 329	26.935	5 90.13	23.876		15.38
30	ATOM	5153	3 C2	A LEU E	3 329	27.178	88.69	9 23.928	1.00	17.98
	ATOM	5154	4 C	3 LEU E	3 329	25.95	9 87.90	8 23.414		17.20
	ATOM	515	5 C	G LEU I	329	24.65	3 88.03	5 24.178		20.30
	ATOM	515	6 C	D1 LEU 1	в 329	23.59	4 87.12	4 23.57	•	21.47
	MOTA	1 515	7 C	D2 LEU	в 329	24.84	5 87.73	1 25.66		22.07
35	OTA 6	· 4 515	8 C	LEU	в 329	28.34	0 88.35	5 23.01	6 1.00	19.84

	ATOM	5159	0	LEU B	329	28.686	89.127	22.097	1.00	24.07
	ATOM	5160	N	THR B	330	28.906	87.177	23.211	1.00	20.62
	MOTA	5161	CA	THR B	330	29.963	86.720	22.333	1.00	20.50
	MOTA	5162	СВ	THR B	330	31.009	85.887	23.065	1.00	20.77
5	ATOM	5163	OG1	THR B	330	.30.442	84.714	23.609	1.00	24.50
	ATOM	5164	CG2	THR B	330	31.752	86.626	24.153	1.00	24.53
	MOTA	5165	C	THR B	330	29.279	85.866	21.262	1.00	18.71
	ATOM	5166	0	THR B	330	28.158	85.406	21.472	1.00	19.35
	MOTA	5167	N	PRO B	331	29.898	85.649	20.099	1.00	19.52
10	ATOM	5168	CD	PRO B	331	31.220	86.162	19.696	1.00	18.68
	MOTA	5169	CA	PRO B	331 .	29.269	84.844	19.046	1.00	18.22
	MOTA	5170	CB _.	PRO B	331	30.390	84.661	18.018	1.00	16.44
	MOTA	5171	CG	PRO B	331	31.249	85.864	18.210	1.00	20.49
	MOTA	5172	С	PRO B	331	28.800	83.506	19.608	1.00	15.48
15	ATOM	5173	0	PRO B	331	27.659	83.139	19.447	1.00	19.60
	ATOM	5174	N	LEU B	332	29.680	82.800	20.290	1.00	18.96
	ATOM	5175	CA	LEU B	332	29.320	81.507	20.885	1.00	21.83
	MOTA	5176	CB	LEU B	332	30.532	80.813	21.489	1.00	22.46
	ATOM	5177	CG	LEU B	332	30.508	79.294	21.410	1.00	24.80
20	ATOM	5178	CD1	LEU B	332	30.219	78.838	19.982	1.00	28.10
	MOTA	5179	CD2	LEU B	332	31.826	78.721	21.909	1.00	27.01
	MOTA	5180	С	LEU B	332	28.190	81.635	21.909	1.00	20.95
	MOTA	5181	0	LEU B	332	27.370	80.737	22.032	1.00	23.46
	MOTA	5182	N	GLU B	333 ·	28.122	82.779	22.599	1.00	21.24
25	MOTA	5183	CA	GLU B	333	27.046	83.035	23.563	1.00	20.71
	MOTA	5184	CB	GLU B	333	27.355	84.274	24.426	1.00	21.87
	MOTA	5185	CG	GLU E	333	28.187	83.989	25.660	1.00	20.42
	ATOM	5186	CD	GLU E	333	28.867	85.226	26.207	1.00	20.58
•	MOTA	5187	OE1	GLU E	333	29.944	85.079	26.817	1.00	24.35
30	MOTA	5188	OE2	GLU E	3 3 3 3	28.341	86.337	26.011	1.00	21.62
	MOTA	5189	С	GLU E	3 3 3 3	25.759	83.284	22.813	1.00	19.41
	MOTA	5190	0	GLU E	3 333	24.691	82.822	23.208	1.00	19.72
	MOTA	5191	N	ALA E	3 334	25.860	84.024	21.707	1.00	20.30
	ATOM	5192	CA	ALA E	3 334	24.676	84.307	20.904	1.00	17.94
35	ATOM	5193	CB	ALA H	3 334	25.014	85.247	19.740	1.00	22.73

	ATOM	5194	С	ALA B 334	24.077	83.000	20.400	1.00 15.00
	ATOM	5195	0	ALA B 334	22.864	82.823	20.414	1.00 15.28
	ATOM	5196	N .	CYS B 335	24.943	82.087	19.956	1.00 16.88
	MOTA	5197	CA	CYS B 335	24.503	80.790	19.439	1.00 19.80
5	ATOM	5198	СВ	CYS B 335	25.712	79.943	18.958	1.00 22.65
	ATOM	5199	SG	CYS B 335	26.495	80.419	17.358	1.00 25.33
	MOTA	5200	С	CYS B 335	23.692	80.022	20.502	1.00 22.56
	ATOM	5201	0	CYS B 335	22.717	79.338	20.177	1.00 23.57
	ATOM	5202	N	ALA B 336	24.109	80.134	21.777	1.00 23.39
10	ATOM	5203	CA	ALA B 336	23.438	79.448	22.891	1.00 22.44
	ATOM	5204	СВ	ALA B 336	24.364	79.323	24.090	1.00 24.40
	ATOM	5205	С	ALA B 336	22.138	80.122	23.300	1.00 22.49
	ATOM	5206	0	ALA B 336	21.348	79.537	24.045	1.00 23.53
	ATOM	5207	N	HIS B 337	21.908	81.351	22.809	1.00 22.20
15	ATOM	5208	CA	HIS B 337	20.690	82.090	23.129	1.00 19.18
	ATOM	5209	CB	HIS B 337	20.677	83.462	22.476	1.00 17.44
	MOTA	5210	CG	HIS .B 337	19.683	84.412	23.083	1.00 12.51
	MOTA	5211	CD	2 HIS B 337	19.854	85.444	23.951	1.00 10.60
	ATOM	. 5212	ND	1 HIS B 337	18.343	84.380	22.799	1.00 12.23
20	ATOM	5213	CE	1 HIS B 337	17.724	85.349	23.456	1.00 11.82
	ATOM	5214	NE	2 HIS B 337	. 18.626	86.009	24.162	1.00 10.75
	ATOM	5215	C	HIS B 337	19.431	81.301	22.787	1.00 23.47
	ATOM	5216	5 0	HIS B 337	19.409	80.490	21.828	1.00 24.86
	MOTA	5217	N	SER B 338	18.391	81.516	23.595	·
25	ATOM	. 5218	3. CA	SER B 338	17.124	80.824	23.446	
	MOTA	5219	e CE	SER B 338	16.243	81.045	24.674	
	MOTA	5220	0 00	SER B 338	15.732	82.352	24.688	
	MOTA	522	1 C	SER B 338	16.375	81.171		
	ATOM	522	2 0	SER B 338	15.437	80.480	21.778	
30	ATOM	522	3 N	PHE B 339	16.800	82.215	21.455	
•	ATOM	522	4 C	A PHE B 339	16.14	4 82.552	2 20.18	
	ATOM	522	5 C	B PHE B 339	16.71	1 83.86	3 19.61	
	MOTA	522	26 C	G PHE B 339	16.17	2 84.23	3 18.25	
	ATOM	522	27 C	D1 PHE B 339	17.03	4 84.53	2 17.20	
35	5 ATOM	1 522	28 C	D2 PHE B 339	14.81	2 84.27	6 18.01	3 1.00 24.61

	MOTA	5229	CE1	PHE E	3	339	16.548	84.868	15.946	1.00	22.40
	MOTA	5230	CE2	PHE E	3 .	339	14.317	84.612	16.761	1.00	24.59
	ATOM	5231	CZ	PHE E	3	339	15.192	84.910	15.727	1.00	21.68
	MOTA	5232	С	PHE E	3	339	16.377	81.398 .	19.193	1.00	21.36
5	ATOM	5233	0	PHE F	3	339	15.579	81.152	18.297	1.00	22.30
	MOTA	5234	N	PHE I	3	340	17.499	80.716	19.386	1.00	21.16
	MOTA	5235	CA	PHE I	3	340	17.941	79.611	18.561	1.00	21.89
	ATOM	5236	СВ	PHE I	3	340 .	19.452	79.723	18.390	1.00	18.67
	ATOM	5237	CG	PHE I	3	340	19.864	81.007	17.720	1.00	17.61
10	ATOM	5238	CD1	PHE I	3	340	19.361	81.342	16.461	1.00	17.37
	ATOM ·	5239	CD2	PHE I	3	340	20.747	81.876	18.331	1.00	16.89
	ATOM	5240	CE1	PHE 1	В	340	19.740	82.517	15.834	1.00	16.28
	MOTA	5241	CE2	PHE 1	В	340	21.131	83.055	17.710	1.00	16.48
	MOTA	5242	CZ	PHE 1	В	340	20.626	83.376	16.456	1.00	16.07
15	MOTA	5243	С	PHE	В	340	17.552	78.222	19.084	1.00	24.76
	MOTA	5244	0	PHE :	В	340	18.009	77.206	18.532	1.00	25.73
	MOTA	5245	N	ASP	В	341	16.699	78.163	20.121	1.00	25.74
	MOTA	5246	CA	ASP	В	341	16.256	76.877	20.674	1.00	26.49
	MOTA	5247	СВ	ASP	В	341	15.383	77.066	21.923	1.00	26.51
20	MOTA	5248	CG	ASP	В	341	16.165	77.514	23.166	1.00	27.55
	MOTA	5249	ODl	ASP	В	341	17.397	77.289	23.232	1.00	24.76
	MOTA	5250	OD2	ASP	В	341	15.535	78.090	24.074	1.00	29.17
	ATOM,	5251	С .	ASP	В	341	15.511	76.037	19:.632	1.00	26.31
	ATOM	5252 [°]	0	ASP	В	341	15.652	74.819	19.599	1.00	27.59
25	MOTA	5253	N	GLU	В	342	14.726	76.693.	18.773	1.00	28.02
	ATOM	5254	CA	GLU	В	342	13.984	75.989	17.723	1.00	27.38
	MOTA	5255	CB	GLU	В	342	13.200	76.983	16.851	1.00	28.41
	ATOM	5256	CG	GLU	В	342	11.835	76.474	16.404	1.00	30.01
	MOTA	5257	CD	GLU	В	342	11.296	77.144	15.141	1.00	30.63
30	MOTA	5258	OE1	GLU	В	342	10.401	76.558	14.499	1.00	33.14
	MOTA	5259	OE2	GLU	В	342	11.755	78.247	14.799	1.00	32.10
	MOTA	5260	С	GLU	В	342	14.936	75.155	16.852	1.00	26.89
	MOTA	5261	0	GLU	В	342	14.623	74.028	16.487	1.00	27.34
	MOTA	5262	N	LEU	В	343	16.104	75.722	16.543	1.00	26.14
35	MOTA	5263	CA	LEU	В	343	17.121	75.056	15.734	1.00	26.03

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	MOTA	5264	CB	LEU B 3	43	18.309	75.995		1.00 2	
	ATOM	5265	CG	LEU B 3	43	18.008	77.353	14.863	1.00	23.80
	ATOM	5266	CD1	LEU B 3	343	19.306	78.029	14.443	1.00	23.33
	ATOM	5267	CD2	LEU B 3	343	17.074	77.199 .	13.670	1.00	23.09
5	ATOM	5268	С	LEU B 3	343	17:622	73.760	16.382	1.00	27.12
	ATOM	5269	0	LEU B 3	343	17.940	72.788	15.681	1.00	26.66
	MOTA	5270	N	ARG B 3	344	17.710	73.753	17.717	1.00	27.38
	MOTA	5271	CA	ARG B 3	344	18.189	72.579	18.461	1.00	28.04
	MOTA	5272	СВ	ARG B 3	344	18.639	72.987	19.873	1.00	26.77
10	ATOM	5273	CG	ARG B 3	344	20.065	73.500	19.918	1.00	23.60
	ATOM	5274	CD	ARG B	344	20.372	74.201	21.229	1.00	20.43
	MOTA	5275	NE	ARG B	344	19.656	75.468	21.370	1.00	15.24
	MOTA	5276	CZ	ARG B	344	20.233	76.664	21.314	1.00	14.32
	ATOM	5277	NHl	ARG B	344	21.514	76.784	21.011	1.00	16.66
15	MOTA	5278	NH2	ARG B	344	19.520	77.750	21.535	1.00	13.81
	ATOM	5279	С	ARG B	344	17:121	71.491	18.533		29.05
	ATOM	5280	0	ARG'B	344	17.413	70.348	18.877	1.00	29.56
	MOTA	5281	N	ASP B	345	15.891	71.847	18.177	1.00	32.04
	MOTA	5282	CA	ASP B	345	14.780	70.905	18.159	1.00	34.68
20	MOTA	5283	CB	ASP B	345	13.523	71.632	17.696	1.00	36.26
	MOTA	5284	CG	ASP B	345	12.250	70.882	17.999	1.00	36.87
	MOTA	5285	ODI	ASP B	345	11.252	71.545	18.346	1.00	40.08
	MOTA	5286	OD2	2 ASP B	345	12.244	69.641	17.877	1:00	38.07
	MOTA	5287	С	ASP B	345	15.116	69.773	17.189	1.00	36.77
25	MOTA	5288	0	ASP B	345	15.513	70.030	16.055	1.00	37.90
	ATOM	5289	N	PRO B	346	15.001	68.509	17.630		38.35
	ATOM	5290	CD	PRO B	346	14.562	68.112	18.980		38.89
	ATOM	5291	CA	PRO B	346	15.342	67.346	16.805		38.95
	MOTĄ	5292	СВ	PRO B	346	15.287	66.185	17.796	1.00	38.46
30	MOTA	5293	CG	PRO B	346	14.329	. 66.639	18.836		38.21
	ATOM	5294	С	PRO B	346	14.379	67.098	15.652	1.00	40.21
	ATOM	5295	0	PRO B	346	14.730	66.413	14.696	1.00	40.40
	MOTA	5296	N	ASN B	3 347	13.171	67.642	15.751	1.00	41.66
	ATOM	5297	CI	A ASN E	3 3 4 7	12.163	67.455	14.712	1.00	43.83
35	MOTA	5298	3 CI	B ASN E	347	10.814	67.114	15.348	1.0	0 45.27
		•								

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	ATOM	5299	CG	ASN	В	347	10.860	65.853	16.188	1.00	46.39
	MOTA	5300	OD1	ASN	В	347	10.326	65.815	17.298	1.00	47.81
	MOTA	5301	ND2	ASN	В	347	11.498	64.811	15.662	1.00	46.93
•	MOTA	5302	С	ASN	В	347	12.017	68.670 .	13.782	1.00	44.37
5 *	ATOM	5303	0	ASN	В	347	11.171	68.666	12.887	1.00	45.46
	ATOM	5304	N	VAL	В	348	12.830	69.706	14.000	1.00	44.26
	ATOM	5305	CA	VAL	В	348	12.770	70.918	13.187	1.00	44.40
	ATOM	5306	CB	VAL	В	348	13:643	72.059	13.765	1.00	43.32
	ATOM	5307	CG1	VAL	В	348	15.106	71.863	13.399	1.00	41.21
10	ATOM	5308	CG2	VAL	В	348	13.146	73.411	13.274	1.00	42.08
	ATOM	5309	С	VAL	В	348	13.151	70.667	11.725	1.00	44.95
	ATOM	5310	.0	VAL	В	348	14.174·	70.043	11.428	1.00	44.90
	ATOM	5311	N	LYS	В	349	12.321	71.178	10.822	1.00	45.79
	MOTA	5312	CA	LYS	В	349	12.554	71.042	9.388	1.00	46.82
15	ATOM ·	5313	.CB	LYS	В	349 .	11.557	70.057	8.758	1.00	48.92
	MOTA	5314	CG	LYS	В	349	11.517	68.692	9.431	1.00	51.59
	MOTA	5315	CD	LYS	В	349	12.587	67.757	8.885	1.00	54.24
	ATOM	5316	CE	LYS	В	349	12.601	66.433	9.638	1.00	56.09
	MOTA	5317	NZ	LYS	В	349	13.905	65.718	9.507	1.00	58.50
20	MOTA	5318	С	LYS	В	349	12.418	72.393	8.700	1.00	46.09
	MOTA	5319	0	LYS	В	349	11.781	73.314	9.227	1.00	45.54
	ATOM	5320	N	LEU	В	350	12.996	72.494	7.507	1.00	45.35
	ATOM	5321	CA	LEU	В	350	12.928	73.709	6.707	1.00	43.22
•	ATOM	5322	CB	LEU	B	350	13.900	73.582	5.535	1.00	43.49
25	ATOM	5323	CG	LEU	В	350	15.222	74.336	5.638	1.00	44.81
	MOTA	5324	CD1	LEU	В	350	15.783	74.263	7.050	1.00	45.17
	MOTA	5325	CD2	LEU	В	350	16.220	73.783	4.625	1.00	43.94
	MOTA	5326	С	LEU	В	350	11.509	73.871	6.156	1.00	41.98
	ATOM	5327	0	LEU	В	350	10.753	72.903	6.117	1.00	42.03
30	MOTA	5328	N	PRO	В	351	11.125	75.090	5.709	1.00	41.39
	ATOM	5329	CD	PRO	В	351	11.947	76.307	5.710	1.00	41.42
	ATOM	5330	CA	PRO	В	351	9.792	75.345	5.145	1.00	41.01
	ATOM	5331	CB	PRO	В	351	9.748	76.866	4.959	1.00	40.02
	MOTA	5332	CG	PRO	B	351	10.909	77.390	5.734	1.00	41.12
35	ATOM	5333	С	PRO	P	351	9.584	74.634	3.802	1.00	40.65

	- = 0\	F334	•	nno p	251	9	.473	74.595	3.286	1.00 4	11.97
	ATOM		•	PRO B ASN B			.646	74.050	3.252	1.00	
	ATOM .	5335		ASN B			.540	73.316	1.988	1.00	
	MOTA	5336	CA CB	ASN B			1.620	73.726	0.976	1.00	
_	MOTA	5337	СБ	ASN B			3.044	73.417	1.414	1.00	
5	ATOM	5338		ASN B			1.001	73.851	0.780	1.00	
4	ATOM	5339		ASN B			3.199	72.672	2.498	1.00	
	ATOM	5340	C C	ASN B		·	0.529	71.798	2.213	1.00	
	ATOM	5341		ASN E			0.550	71.024	1.255	1.00	
10	ATOM	5342	•	GLY E		-	0.475	71.382	3.492		45.59
10	ATOM	5343	N				0.430	69.962	3.839		45.61
	ATOM	5344	CA	GLY E			1.785	69.334	4.108		45.64
	ATOM	5345	C	GLY F		·	1.890	68.383	4.888		45.91
	ATOM	5346	0	GLY I	\		2.818	69.845	3.450		45.87
1: 5	ATOM	5347	N	ARG I			4.168	69.320	3.607		46.82
15	ATOM	5348	CA		B 354		5.118	70.022	2.642		48.66
	ATOM	5349	CB	•	B 354		5.879	69.068	1.739		51.69
	ATOM	5350	CG	· ARG			6.789	69.826	0.782		54.15
	ATOM	5351	CD		B 354		6.023	70.611	-0.188		55.74
20	MOTA	5352	NE		B 354		6.471	70.956	-1.402		56.23
20	ATOM	5353	CZ		B 354		17.690	70.599	-1.806		55.16
	ATOM	5354	NH]		B 354		15.693	71.668	-2.210		56.28
	ATOM	5355	NH2		B 354		14.677	69.490	5.036		45.85
	ATOM	5356	C.		B 354		14.109		5.824		46.19
0.5	ATOM	5357	0		B 354		15.763		5.354		44.37
25	MOTA	5358	N		B 355		16.369	1 1	6.680	-	43.25
	ATOM	5359			B 355		17.386		6.896		43.57
	ATOM	5360			B 355		16.791		6.930		44.36
	ATOM	5361					17.545		6.667		43.84
20	MOTA	5362			B 355		15.584		7.229		46.22
30	MOTA	5363		•	B 355				6.820		41.99
	MOTA	5364			B 355		17.118		5.821		41.58
	MOTA				B 355		17.510				39.86
	MOTA				B 356		17.35			•	36.95
	MOTA				. в 356		18.100				36.53
35	MOTA	536	B CI	3 THR	В 356	•	18.01	6 72.233	9.762	1.01	, ,,,,,

	ATOM	5369	OG1	THR	В	356	18.489	71.203	10.615	1.00	35.15
	MOTA	5370	CG2	THR	В	356	16.626	72.620	10.205	1.00	34.96
	MOTA	.5371	C.	THR	В	356 .	19.543	71.548	7.930	1.00	35.17
	ATOM	5372	0	THR	В	356	20.012	70.418	8.058	1.00	34.12
5	ATOM	537.3	N	PRO	В	357	20.272	72.576	7.484	1.00	34.19
	ATOM	5374	CD	PRO	В	357	19.788	73.953	7.304	1.00	33.98
	ATOM	5375	CA	PRO	В	35 ⁷	21.680	72.425	7.131	1.00	34.20
	ATOM	5376	CB	PRO	В	357	22.115	73.845	6.729	1.00	34.84
•	ATOM	5377	CG	PRO	В	357	21.057	74.755	7.256	1.00	34.63
10	ATOM	5378	С	PRO	В	357	22.496	71.937	8.331	1.00	35.28
•	MOTA	5379	0	PRO	В	357	21.939	71.558	9:371	1.00	35.46
	MOTA	5380	N .	ALA	В	358	23.812	71.957	8.189	1.00	34.83
	ATOM	5381	CA	ALA	В	358	24.707	71.525	9.251	1.00	35.70
	ATOM	5382	CB	ALA	В	358	26.117	71.327	8.712	1.00	35.68
15	ATOM	5383	С	ALA	В	358	24.728	72.501	10.437	1.00	36.22
	MOTA	5384	0	ALA	В	358	24.979	73.702	10.285	1.00	37.18
	MOTA	5385	N	LEU	В	359	24.505	71.945	11.612	1.00	34.98
	MOTA	5386	CA	LEU	В	359	24.526	72.662	12.886	1.00	35.55
	MOTA	5387	CB	LEU	В	359	23.135	73.171	13.288	1.00	34.14
20	MOTA	5388	CG	LEU	В	359	22.245	73.728	12.175	1.00	35.54
	MOTA	5389	CD1	LEU	В	359	20.775	73.629	12.559	1.00	35.56
•	MOTA	5390	CD2	LEU	В	359	22.617	75.169	11.852	1.00	35.80
	ATOM	5391	С	LEU	В	359	25.024	71.670	13.922	1.00	36.61
	ATOM	5392	0	LEU	В	359	24.878	70.459	13.719	1.00	39.28
25	ATOM	5393	N	PHE	В	360	25.618	72.151	15.014	1.00	35.74
	MOTA	5394	CA	PHE	В	360	26.140	71.244	16.070	1.00	34.10
•	MOTA	5395	CB	PHE	В	360	25.101	70.202	16.508	1.00	29.33
	MOTA	5396	CG	PHE	В	360	23.680	70.666	16.405	1.00	26.36
	MOTA	5397	CD1	PHE	В	360	22.752	69.925	15.695	1.00	23.97
30	MOTA	5398	CD2	PHE ·	В	360	23.275	71.847	17.005	1.00	24.93
	MOTA	5399	CE1	PHE	В	360	21.446	70.351	15.579	1.00	21.97
	MOTA	5400	CE2	PHE	В	360	21.969	72.277	16.896	1.00	22.81
	ATOM	5401	CZ	PHE	В	360	21.051	71.525	16.180	1.00	22.58
	ATOM	5402	С	PHE	В	360	27.437	70.555	15.638	1.00	33.93
35	MOTA	5403	0	PHE	В	360	28.007	69.749	16.371	1.00	33.19

	ATOM	5404	N	ASN B	361	27.899	70.912	14.447	1.00 [.] 34	.31
	ATOM	5405	CA	ASN B	361	29.133	70.399	13.858	1.00 34	.36
	ATOM	5406	СВ	ASN B	361	29.057	70.666	12.340	1.00 36	5.65
	MOTA	5407	CG	ASN B	361	29.837	69.677	11.501	1.00 40	0.02
5	ATOM.	5408	OD1	ASN B	361	29.922	68.485	11.828	1.00 40	0.13
	ATOM	5409	ND2	ASN B	361	30.414	70.171	10.402	1.00 43	L.04
	ATOM	5410	С	ASN B	361	30.330	71.154	14.458	1.00 33	3.34
	MOTA	5411	0	ASN B	361	31.319	71.430	13.774	1.00 3	1.51
	ATOM	5412	N	PHE B	362	30.196	71.521	15.743	1.00 3	1.80
10	ATOM	5413	CA	PHE B	362	31.196	72.289	16.496	1.00 2	8.71
	MOTA	5414	СВ	PHE E	362	30.653	72.660	17.886	1.00 2	6.16
	MOTA	5415	CG	PHE E	3 362	29.640	73.763	17.848	1.00 2	2.34
	ATOM	5416	CD1	. PHE E	3 362	28.290	73.482	17.918	1.00 2	2.56
	MOTA	5417	CD2	PHE E	3 3 6 2	30.042	75.081	17.724	1.00 2	2.48
15	ATOM	5418	CE1	PHE I	362	27.356	74.496	17.867	1.00 2	2.49
	MOTA	5419	CE2	2 PHE I	B 362	29.118	76.099	17.673	1.00 1	9.68
	ATOM	5420	CZ	PHE 1	B 362	27.775	75.807	17.744	1.00 2	1.78
	MOTA	5421	С	PHE 1	в 362	32.537	71.591	16.625	1.00 2	27.92
	ATOM	5422	0	PHE	в 362	32.612	70.376	16.705	1.00 2	29.45
20	ATOM	5423	N	THR	в 363	33.601	72.388	16.658	1.00 2	29.26
	ATOM	5424	CA	THR	в 363	34.954	71.859	16.783	1.00	30.32
	MOTA	542 5	СВ	THR	в 363	35.778	72.296	15.582	1.00 2	29.40
	MOTA	5426	OG	1 THR	в 363	37.077	71.754	15.666	1.00	32.75
	ATOM	5427	CG	2 THR	В 363	35.928	73.795	15.485	1.00	29.08
25	ATOM	5428	С	THR	В 363	35.681	72.362	18.034	1.00	30.21
	ATOM ·	.5429	· 0	THR	B 363	35.297	73.357	18.643	1.00	28.68
	ATOM	5430) N	THR	B 364	36.794	71.687	18.336	1.00	32.03
	ATOM	5431	_ C?	A THR	в 364	37.682	72.050	. 19.433	1.00	33.02
	MOTA	5432	2 CI	3 THR	В 364	38.534	70.857	19.866	1.00	30.93
30	ATOM	5433	3 00	G1 THR	в 364	37.735	69.764	20.246	1.00	30.53
	ATOM	543	4 C	G2 THR	в 364	39.494	71.166	20.993	1.00	33.47
	MOTA	543	5 C	THR	В 364	38.59	6 73.166	18.942	1.00	34.09
	ATOM	543	6 0	THR	В 364	39.75	7 72.94	18.578	1.00	35.92
	ATOM	543	7 N	GLN	в 365	38.03	2 74.35	3 18.916	1.00	33.64
35	ATOM	543	8 C	A GLN	в 365	38.68	2 · 75.57	8 18.468	1.00	31.88

	ATOM	5439	СВ	GLN	В	365	39.393	75.369	17.119	1.00	32.40
	ATOM	5440 ·	CG	GLN	В	365	39.723	76.653	16.360	1.00	30.97
	MOTA.	5441	CD	GLN	В	365	41.069	77.252	16.737	1.00	30.44
	ATOM	5442	OE1	GLN	В	365	41.166	78.439 .	17.028	1.00	31.75
5	MOTA	5443	NE2	GLN	B	365	42.112	76.438	16.726	1.00	30.94
	ATOM	5444	С	GLN	В	365	37.591	76.627	18.360.	1.00	29.09
	MOTA	5445	0	GLN	В	365	37.726	77.748	18.841	1.00	30.36
	ATOM	5446	N	GLU	В	366	36.486	76.205	17.772	1.00	26.33
	ATOM	5447	CA	GLU	B	366	35.306	77.026	17.614	1.00	26.16
10	ATOM.	5448	CB	GLU	В	366 `	34.363	76.313	16.636	1.00	24.51
•	ATOM	5449.	CG	GLU	В	366	33.272	77.179	16.026	1.00	22.75
	MOTA	5450	CD	GLU	В	366	32.249	76.358	15.262	1.00	20.28
	ATOM	5451	OE1	GLU	В	366	31.130	76.851	1.5.057	1.00	21.44
	ATOM	5452	OE2	GLU	B	366	32.564	75.215	14.880	1.00	21.96
15	ATOM	5453	С	GLU	В	366	34.602	77.195	18.969	1.00	26.22
	ATOM	5454	0	GLU	В	366	33.842	78.137	19.172	1.00	26.02
	ATOM .	5455	N	LEU	В	367	34.857	76.257	19.884	1.00	27.86
•	ATOM	5456	CA	LEU	В	367	34.251	76.269	21.217	1.00	28.45
	ATOM	5457	CB	LEU	В	367	33.839	74.840	21.631	1.00	26.52
20	ATOM .	5458	CG	LEU	В	367	32.727	74.155	20.818	1.00	24.71
	MOTA	5459	CD1	LEU	В	367	32.726	72.654	21.075	1.00	23.77
	MOTA	5460	CD2	LEU	В	367	31.362	74.745	21.135	1.00	24.85
	ATOM	5461	С	LEU	В	367	35.209	76.829	22.272	1:00	29.25
	ATOM	5462	0	LEU	В	367	34.798	77.109	23.393	.1.00	28.89
25	MOTA	5463	N	SER	В	368	36.484	76.941	21.906	1.00	29.41
	ATOM	5464	CA	SER	В	368	37.565	77.401	22.778 -	1.00	31.33
	ATOM	5465	CB	SER	В	368	38.843	77.631	21.971	1.00	32.29
	ATOM	5466	OG	SER	В	368	38.695	78.719	21.073	1.00	35.8 ⁷
	ATOM	5467	C	SER	В	368	37.260	78.613	23.675	1.00	32.52
30	MOTA	5468	0	SER	В	368	37.822	78.722	24.774	1.00	34.50
	ATOM	5469	N	SER	В	369	36.418	79.531	23.219	1.00	31.73
	MOTA	5470	CA	SER	В	369	36.107	80.729	24.006	1.00	30.54
	MOTA	5471	CB	SER	В	369	35.446	81.806	23.140	1.00	27.93
	MOTA	5472	OG	SER	В	369	34.055	81.585	23.014	1.00	26.02
35	ATOM	5473	С	SER	В	369	35.266	80.427	25.252	1.00	31.02

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		LI		.5 / U	34.632	19.200	25.268	1.00 3	0.60
MION	5476				33.788	78.823	26.377	1.00 2	9.03
η TPOM		•				79.707	. 26.453	1.00 3	80.95
						79.694	27.826	1.00 3	30.19
					31.168	80.623	28.197	1.00 3	30.56
					32.114	78.638	28.578	1.00 3	30.43
					33.385	77.352	/26.220	1.00 2	26.71
		_			32.225	77.050	25.969	1.00 2	29.86
					34.347	76.419	26.352	1.00	25.41
				•	35.765	76.702	26.633	1.00	25.72 .
					34.116	74.969	26.203	1.00	26.79
	•				35.322	74.361	26.903	1.00	26.64
			PRO E	371	36.410	75.338	26.630	1.00	26.89
		C	PRO. H	371	32.790	74.423	26.776	1.00	28.36
		0	PRO I	371	32.100	73.658	26.100	1.00	29.50
	5490	N	PRO I	в 372	32.419	74.758	28.031	1.00	29.03
	5491	CD	PRO 1	B 372	33.178	75.609	28.965	1.00	29.71
	5492	CA	PRO !	в 372	31.180	74.249	28.638	1.00	29.24
ATOM	5493	СВ	PRO :	в 372	31.158	74.870	30.042	1.00	29.18.
MOTA	5494	CG	PRO	в 372	32.154	75.980	30.002	1.00	31.38
MOTA	5495	С	PRO	в 372	29.912	74.625	27.864	1.00	28.57
MOTA	5496	0	PRO	в 372	28.876	73.977	28.015	1:00	29.72
ATOM	5497	N	LEU	в 373	29.978	75.670	27.042	1.00	28.85
ATOM	5498	CA	LEU	в 373	28.798	76.08	26.276	1.00	28.73
MOTA	5499	СВ	LEU	в 373	29.055	77.37	3 25.481	1.00	28.83
MOTA	5500	ÇG	LEU	B 373	28.932	78.68	1 26.272	1.00	29.03
MOTA	5501	CD	1 LEU	в 373	29.170	79.89	25.376		27.64
ATOM	5502	CD	2 LEU	в 373	27.577	78.78	1 26.959	1.00	29.15
ATOM	5503	C	LEU	в 373	28.266	74.95	7 25.387	1.00	27.06
MOTA	5504	. 0	LEU	в 373	27.118	74.98	6 24.956	1.00	27.47
ATOM	5505	S N	ALA	В 374	29.099	9 73.94	6 25.161	1.00	27.71
ATOM	5506	5 CF	ALA	в 374	28.73	1 72.77	4 24.367		29.52
ATOM	550	7 CI	3 ALA	В 374	29.91	2 71.82	8 24.238		28.86
ATOM	550	в с	ALA	в 374	27.52	0 72.02	29 24.93	5 1.00	30.78
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 5477 ATOM 5478 ATOM 5479 ATOM 5480 ATOM 5481 ATOM 5482 ATOM 5483 ATOM 5484 ATOM 5485 ATOM 5486 ATOM 5488 ATOM 5488 ATOM 5489 ATOM 5490 ATOM 5491 ATOM 5492 ATOM 5493 ATOM 5493 ATOM 5494 ATOM 5495 ATOM 5496 ATOM 5497 ATOM 5498 ATOM 5497 ATOM 5498 ATOM 5497 ATOM 5498 ATOM 5498 ATOM 5499 ATOM 5500 ATOM 5501 ATOM 5502 ATOM 5503 ATOM 5503 ATOM 5503	ATOM 5477 CB ATOM 5478 CG ATOM 5479 OD1 ATOM 5480 ND2 ATOM 5481 C ATOM 5482 O ATOM 5483 N ATOM 5484 CD ATOM 5485 CA ATOM 5486 CB ATOM 5489 O ATOM 5490 N ATOM 5491 CD ATOM 5492 CA ATOM 5493 CB ATOM 5494 CG ATOM 5495 C ATOM 5496 O ATOM 5497 N ATOM 5498 CA ATOM 5499 CB ATOM 5499 CB ATOM 5499 CB ATOM 5500 CG ATOM 5501	ATOM 5477 CB ASN B ATOM 5478 CG ASN B ATOM 5479 OD1 ASN B ATOM 5480 ND2 ASN B ATOM 5481 C ASN B ATOM 5482 O ASN B ATOM 5483 N PRO B ATOM 5484 CD PRO B ATOM 5486 CB PRO B ATOM 5488 C PRO B ATOM 5489 O PRO B ATOM 5491 CD PRO B ATOM 5492 CA PRO B ATOM 5493 CB PRO ATOM 5494 CG PRO ATOM 5495 C PRO ATOM 5496 O PRO ATOM	ATOM 5477 CB ASN B 370 ATOM 5478 CG ASN B 370 ATOM 5480 ND2 ASN B 370 ATOM 5481 C ASN B 370 ATOM 5482 O ASN B 370 ATOM 5483 N PRO B 371 ATOM 5484 CD PRO B 371 ATOM 5486 CB PRO B 371 ATOM 5488 C PRO B 371 ATOM 5489 C PRO B 371 ATOM 5489 C PRO B 372 ATOM 5491 CD PRO B 372 ATOM 5494 CG PRO B 372 ATOM 5494 CG PRO B 372 ATOM 5494 CG PRO B 372 ATOM 5495 C PRO B 372 ATOM 5496 CB PRO B 372 ATOM 5497 N PRO B 372 ATOM 5498 CA PRO B 373 ATOM 5499 CB LEU B 373 ATOM 5490 CG LEU B 373 ATOM 5490 CG LEU B 373 ATOM 5491 CD PRO B 372 ATOM 5494 CG PRO B 372 ATOM 5495 C PRO B 372 ATOM 5496 O PRO B 372 ATOM 5496 C PRO B 373 ATOM 5497 N LEU B 373 ATOM 5498 CA LEU B 373 ATOM 5500 CG LEU B 373 ATOM 5501 CD1 LEU B 373 ATOM 5502 CD2 LEU B 373 ATOM 5504 O LEU B 373 ATOM 5505 N ALA B 374 ATOM 5506 CA ALA B 374 ATOM 5506 CA ALA B 374	ATOM 5477 CB ASN B 370 32.537 ATOM 5478 CG ASN B 370 31.882 ATOM 5480 ND2 ASN B 370 32.114 ATOM 5481 C ASN B 370 32.225 ATOM 5482 O ASN B 370 32.225 ATOM 5484 CD PRO B 371 35.765 ATOM 5486 CB PRO B 371 35.322 ATOM 5487 CG PRO B 371 36.410 ATOM 5488 C PRO B 371 32.790 ATOM 5490 N PRO B 372 32.419 ATOM 5491 CD PRO B 372 32.419 ATOM 5494 CG PRO B 372 31.180 ATOM 5495 C PRO B 372 32.154 ATOM 5496 C PRO B 372 32.154 ATOM 5496 C PRO B 372 32.154 ATOM 5497 N LEU B 373 29.912 ATOM 5498 CA LEU B 373 29.912 ATOM 5499 CB LEU B 373 29.978 ATOM 5499 CB LEU B 373 29.978 ATOM 5499 CB LEU B 373 29.978 ATOM 5500 CG LEU B 373 29.978 ATOM 5501 CD1 LEU B 373 29.978 ATOM 5503 C LEU B 373 29.978 ATOM 5504 O LEU B 373 27.1180 ATOM 5505 N ALA B 374 29.991	ATOM 5477 CB ASN B 370 32.537 79.707 ATOM 5478 CG ASN B 370 31.882 79.694 ATOM 5479 OD1 ASN B 370 31.168 80.623 ATOM 5480 ND2 ASN B 370 32.114 78.638 ATOM 5481 C ASN B 370 32.225 77.050 ATOM 5482 O ASN B 370 32.225 77.050 ATOM 5484 CD PRO B 371 34.347 76.419 ATOM 5485 CA PRO B 371 34.316 74.969 ATOM 5486 CB PRO B 371 35.322 74.361 ATOM 5487 CG PRO B 371 36.410 75.338 ATOM 5489 O PRO B 371 32.790 74.423 ATOM 5489 C PRO B 371 32.100 73.658 ATOM 5490 N PRO B 372 32.419 74.758 ATOM 5491 CD PRO B 372 32.419 74.758 ATOM 5492 CA PRO B 372 31.180 74.249 ATOM 5493 CB PRO B 372 31.158 74.870 ATOM 5494 CG PRO B 372 32.154 75.980 ATOM 5495 C PRO B 372 32.154 75.980 ATOM 5496 O PRO B 372 32.154 75.980 ATOM 5497 N LEU B 373 29.912 74.625 ATOM 5499 CB LEU B 373 29.978 75.670 ATOM 5499 CB LEU B 373 29.978 75.670 ATOM 5500 CG LEU B 373 29.978 75.670 ATOM 5501 CD1 LEU B 373 29.978 76.981 ATOM 5503 C LEU B 373 27.577 78.78 ATOM 5504 O LEU B 373 27.577 78.78 ATOM 5505 N ALA B 374 29.999 73.94 ATOM 5506 CA ALA B 374 29.999 73.94 ATOM 5506 CA ALA B 374 29.999 73.94 ATOM 5507 CB ALA B 374 29.999 73.94	ATOM 5476 CB ASN B 370 32.537 79.707 26.453 ATOM 5479 ODL ASN B 370 31.882 79.694 27.826 ATOM 5480 ND2 ASN B 370 32.114 78.638 28.578 ATOM 5481 C ASN B 370 32.114 78.638 28.578 ATOM 5482 O ASN B 370 32.225 77.050 25.969 ATOM 5483 N PRO B 371 34.347 76.419 26.352 ATOM 5484 CD PRO B 371 35.765 76.702 26.633 ATOM 5485 CA PRO B 371 36.410 75.338 26.630 ATOM 5486 CB PRO B 371 36.410 75.338 26.630 ATOM 5489 O PRO B 371 32.790 74.423 26.776 ATOM 5490 N PRO B 372 32.419 74.758 28.031 ATOM 5491 CD PRO B 372 33.178 75.609 28.965 ATOM 5492 CA PRO B 372 31.158 74.870 30.042 ATOM 5493 CB PRO B 372 31.158 74.870 30.042 ATOM 5494 CG PRO B 372 31.158 74.870 30.042 ATOM 5495 C PRO B 372 32.154 75.980 30.002 ATOM 5496 O PRO B 372 32.154 75.980 30.002 ATOM 5497 N LEU B 373 29.912 74.625 27.864 ATOM 5498 CA LEU B 373 29.978 75.670 27.042 ATOM 5499 CB LEU B 373 29.978 75.670 27.042 ATOM 5509 CG LEU B 373 29.978 75.670 27.042 ATOM 5500 CG LEU B 373 29.978 75.670 27.042 ATOM 5500 CG LEU B 373 29.979 73.946 25.161 ATOM 5500 CG LEU B 373 29.909 73.946 25.161 ATOM 5500 CG LEU B 373 29.909 73.946 25.161	ATOM 5477 CB ASN B 370 32.537 79.707 26.453 1.00 3 ATOM 5478 CG ASN B 370 31.882 79.694 27.826 1.00 3 ATOM 5479 OD1 ASN B 370 31.168 80.623 28.197 1.00 3 ATOM 5480 ND2 ASN B 370 32.114 78.638 28.578 1.00 3 ATOM 5481 C ASN B 370 32.225 77.050 25.969 1.00 3 ATOM 5482 O ASN B 370 32.225 77.050 25.969 1.00 3 ATOM 5483 N PRO B 371 34.347 76.419 26.352 1.00 3 ATOM 5484 CD PRO B 371 34.347 76.419 26.352 1.00 3 ATOM 5485 CA PRO B 371 34.116 74.969 26.203 1.00 3 ATOM 5486 CB PRO B 371 35.322 74.361 26.903 1.00 3 ATOM 5487 CG PRO B 371 35.322 74.361 26.903 1.00 3 ATOM 5488 C PRO B 371 32.790 74.423 26.776 1.00 3 ATOM 5489 O PRO B 371 32.100 73.658 26.100 1.00 3 ATOM 5490 N PRO B 372 32.419 74.758 28.031 1.00 3 ATOM 5491 CD PRO B 372 33.178 75.609 28.965 1.00 3 ATOM 5492 CA PRO B 372 31.180 74.249 28.638 1.00 3 ATOM 5494 CG PRO B 372 31.158 74.870 30.042 1.00 3 ATOM 5495 C PRO B 372 32.154 75.980 30.002 1.00 3 ATOM 5496 O PRO B 372 32.154 75.980 30.002 1.00 3 ATOM 5497 N LEU B 373 29.972 74.625 27.864 1.00 3 ATOM 5498 CA LEU B 373 28.876 73.977 28.015 1.00 3 ATOM 5499 CB LEU B 373 28.975 77.373 25.481 1.00 3 ATOM 5499 CB LEU B 373 28.975 77.373 25.481 1.00 3 ATOM 5500 CG LEU B 373 28.975 77.373 25.481 1.00 3 ATOM 5501 CD1 LEU B 373 28.975 77.373 25.376 1.00 3 ATOM 5502 CD2 LEU B 373 28.266 74.957 25.376 1.00 3 ATOM 5504 O LEU B 373 28.266 74.957 25.376 1.00 3 ATOM 5505 N ALA B 374 29.099 73.946 25.161 1.00 3 ATOM 5507 CB ALA B 374 29.099 73.946 25.161 1.00 3 ATOM 5507 CB ALA B 374 29.099 73.946 25.161 1.00 3 ATOM 5507 CB ALA B 374 29.099 73.946 25.161 1.00 3

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	ATOM	5509	0	ALA B	374	26.806	71.353	24.190	1.00	30.95
	MOTA	5510	И	THR B	375	27.279	72.143	26.252	1.00	31.43
	MOTA	5511	CA	THR B	375	26.133	71.454	26.868	1.00	31.02
	ATOM	5512	СВ	THR B	375	26.130	71.567 .	28.406	1.00	31.88
5	ATOM	5513	OG1	THR B	375	26.135	72.915	28.829	1.00	33.01
	ATOM	5514.	CG2	THR B	375	27.283	70.861	29.079	1.00	30.87
	ATOM	5515	С	THR B	375	24.809	71.933	26.288	1.00	29.69
	ATOM	5516	0	THR B	375	23.835	71.185	26.234	1.00	29.64
	ATOM	5517	N	ILE B	376	24.780	73.177	25.846	1.00	30.31
10	ATOM	5518	CA	ILE B	376	23.577	73.754	25.254	1.00	30.34
	ATOM	5519	CB	ILE B	376	23.427	75.236	.25.645	1.00.	31.90
	ATOM	5520	CG2	TLE B	376	22.130	75.811	25.093	1.00	33.49
	ATOM	5521	CG1	ILE B	376	23.494	75.418	27.166	1.00	33.13
	ATOM	5522	CD1	ILE B	376	23.394	76.865	27.603	1.00	30.17
15	MOTA	5523	C	ILE B	376	23.648	73.672	23.720	1.00	29.48
	MOTA	5524	0	ILE B	376	22.706	73.231	23.063	1.00	28.38
	ATOM	5525	N	LEU B	377	24.780	74.123	23.182	1.00	29.90
	MOTA	5526	CA	LEU B	377	25.057	74.163	21.746	1.00	29.31
	MOTA	5527	CB	LEU B	377	26.473	74.667	21.509	1.00	27.56
20	MOTA	5528	CG	LEU. B	377 ·	26.729	76.105	21.953	1.00	25.82
	MOTA	5529	CD1	LEU B	377 .	28.185	76.483	21.739	1.00	24.88
	MOTA	5530	CD2	LEU B	377	25.799	77.061	21.225	1.00	25.71
	ATOM	5531 [.]	С	LEU B	377	24.838	72.828	21.054	1.00	29.70
	MOTA	5532	. O	LEU B	377	24.192	72.776	20.019	1.00	30.42
25	MOTA	5533	N	ILE B	378	25.363	71.754	21.643	1.00	30.75
	MOTA	5534	CA	ILE B	. 378	25.211	70.413	21.097	1.00	30.50
	MOTA	5535	CB	ILE B	378	26.559	69.669	21.074	1.00	30.22
	MOTA	5536	CG2	ILE B	378	26.400	68.295	20.428	1.00	30.35
	MOTA	5537	CG1	ILE E	378	27.607	70.511	20.323	1.00	28.02
30	MOTA	5538	CD1	ILE E	378	29.016	69.974	20.416	1.00	27.08
	ATOM	5539	С	ILE E	3 378	24.173	69.605	21.882	1.00	32.15
	MOTA	5540	0	ILE F	3 378	24.491	68.998	22.905	1.00	33.58
	ATOM	. 5541	N	PRO E	379	22.908	69.598	21.418	1.00	32.79
	MOTA	- 5542	CD	PRO P	379	22.434	70.307	20.215	1.00	34.93
35	ATOM	5543	CA	PRO E	3 379	21.819	68.875	22.084	1.00	33.56

									•	
	ATOM	554 [.] 4	СВ	PRO B	379	20.581	69.214	21.244	1.00 33	
	ATOM	5545	CG	PRO B	379	21.127	69.633	19.922	1.00 34	
	ATOM	5546	C	PRO B	379	22.053	67.369	22.126	1.00 33	
	MOTA	5547	0	PRO B	379	22.885	66.844	21.385	1.00 34	
5	ATOM	5548	N	PRO B	380	21,328	66.659	23.020	1.00 33	
	ATOM	5549	CD	PRO B	380	20.333	67.233	23.959	1.00 34	.16
	ATOM	5550	CA	PRO B	380	21.458	65.197	23.196	1.00 33	
	ATOM	5551	СВ	PRO B	380	20.300	64.850	24.139	1.00 33	
	ATOM	5552	CG	PRO B	380	20.072	66.100	24.917	1.00 34	
10	ATOM	5553	С	PRO B	380	21.338	64.405	21.890	1.00 33	
	ATOM	5554	0	PRO B	380	22.153	63.528	21.617	1.00 3	
	MOTA	5555	N	HIŞ B	381	20.320	64.713	21.096	1.00 3	
	ATOM	5556	CA	HIS B	381	20.081	64.027	19.825	1.00 3	
	ATOM	5557	СВ	HIS B	381	18.759	64.499	19.210	1.00 3	
15	ATOM	5558	CG	HIS B	381	18.812	65.874	18.604	1.00 3	
	ATOM	5559	CD	2 HIS E	3 381	18.392	67.070	19.077	1.00 3	
	ATOM	5560	ND	l HIS E	3 381	19.341	66.129		1.00 3	
	ATOM	5561	. CE	1 HIS B	3 381	19.246	67.420		1.00 3	
	MOTA	5562	NE	2 HIS H	B 381	18.673	68.013	18.115		
20	ATOM.	5563	3 C	HIS !	B 381	21.221	64.215			
	ATOM	5564	1 0	HIS	B 381	21.357	63.427			
	MOTA	556	5 N	ALA	В 382	22.013	65.273	3 19.002		
	MOTA	556	6 C	A ALA	B 382	23.119	65.594	•		
	MOTA	556	7 C	B ALA	B 382	23.175	67.09	7 17.866		
25	MOTA	556	8 C	ALA	В 382	24.473	65.09			42.29
	MOTA	556	9 . 0	ALA	B 382	25.485	65.30			41.80
	ATOM	557	0 N	ARG	B 383	24.504				43.81
	ATOM	557	1 0	A ARG	B 383	25.757	7 63.94			46.02
	MOTA	557	2 0	B ARG	B 383	25.71	1 63.94		0.	44.99
30) ATOM	55	73 (CG ARG	B 383	25.91	1 65.32	•		42.60
• •	ATOM	1 55	74 (CD ARG	B 383	25.62	9 65.32			41.32
	MOTA	4. 55	75 I	NE ARG	В 383	25.02			•	40.35
	ATO	<u>4</u> 55	76	CZ ARG	B 383	24.25	9 66.72	20 25.45		38.67
	ATO	M 55	77	NH1 ARG	B 383	24.01	.4 65.6			37.27
3	5 ATO	M 55	78	NH2 ARC	3 B 383	23.74	67.9	08 25.75	51 1.00	36.51

	MOTA	5579	С	ARG	В	383	2	6.062	62.533	19.788	1.00	48.67
	MOTA	5580	0	ARG	В	383	2	5.150	61.745	19.516	1.00	49.21
	ATOM	5581	N	ILE	В	384	2	7.355	62.223	19.671	1.00	51.03
	ATOM	5582	CA	ILE	В	384	2	7.798	60.910	.19.205	1.00	52.96
5	ATOM	5583	CB	ILE	В	384	2	8.920	61.013	18.148	1.00	52.76
	ATOM	5584	CG2	ILE	В	384	2	9.157	59.658	17.496	1.00	52.75
•	ATOM	5585	CG1	ILE	В	384	2	8.563	62.059	17.086	1.00	51.93
	ATOM	5586	CD1	ILE	В	384	2	9.492	63.253	17.068	1.00	51.77
	ATOM	5587	С	ILE	В	384	2	8.272	60.041	20.372	1.00	54.86
10	ATOM	5588	OT1	ILE	В	38.4	2	8.001	58.815	20.344	1.00	55.31
•	ATOM	5589	OXT	ILE	В	384	2	8.909	60.593	21, 309	1.00	55.89
	TER	5590	•	ILE	В	384			•			
	MOTA	5591	OH2	TIP		1	. 2	20.184	97.209	9.978	1.00	14.30
	MOTA	5592	OH2	TIP		2	8	86.592	49.067	10.183	1.00	15.43
15	MOTA	5593	OH2	TIP		3	1	.7.055	66.016	22.246	1.00	16.08
	MOTA	5594	OH2	TIP		4	4	13.676	99.232	10.734	1.00	18.27
•	ATOM	5595	OH2	TIP	•	5	7	4.057	43.510	23.648	1.00	8.65
	ATOM	5596	OH2	TIP		6	7	79.150	41.199	7.662	1.00	16.64
	MOTA	5597	OH2	TIP		7	7	73.604	48.334	14.257	1.00	17.10
20	MOTA	5598	OH2	TIP		8	7	71.710	51.582	3.800	1.00	26.80
	MOTA	5599	OH2	TIP		9	-	74.647	44.648	12.301	1.00	25.74
	MOTA	5600	OH2	TIP		10	6	58.184	50.139	5.114	1.00	22.46
	ATOM	5601	OH2	TIP		11	3	30.995	97.272	13.532	1.00	24.09
	ATOM ·	5602	OH2	TIP		12	3	31.473	94.065	11.111	1.00	35.85
25	ATOM	5603	OH2	TIP		13	8	38.665	47.357	16.164	1.00	21.52
	ATOM	5604	OH2	TIP		14	(62.931	47.153	11.083	1.00	15.13
	MOTA	5605	OH2	TIP		15		32.589	83.518	20.788	1.00	21.19
	ATOM	5606	OH2	TIP		16	•	76.928	36.781	1.256	1.00	35.32
	MOTA	5607	OH2	TIP		17	•	77.542	40.357	22.692	1.00	20.20
30	MOTA	5608	OH2	TIP		18	•	39.998	74.585	11.864	1.00	33.26
	ATOM	5609	OH2	TIP	•	19	•	75.908	25.776	8.313	1.00	31.07
	MOTA	5610	OH2	TIP	•	20		36.308	91.732	5.629	1.00	20.75
	ATOM	5611	OH2	TIP)	21		34.229	87.485	20.266	1.00	30.78
	ATOM	5612	OH2	TIP	•	22		69.815	37.826	0.045	1.00	31.95
35	MOTA	5613	OH2	TIP	•	23		78.149	47.463	24.796	1.00	15.46

	ATOM	5614	OH2 TIP	24	67.941	51.729	13.432	1.00 17.40
	ATOM	.5615	OH2 TIP	25	69.556	26.809	16.650	1.00 25.99
	ATOM	5616	OH2 TIP	26	82.058	56.569	8.529	1.00 32.89
	ATOM	5617	OH2 TIP	27	34.979	82.693	19.866	1.00 23.31
5	ATOM	5618	OH2 TIP	28	23.280 1	100.047	25.484	1.00 24.88
	MOTA	5619	OH2 TIP	29	35.288	97.692	5.905	1.00 22.00
	ATOM	5620	OH2 TIP	30 .	76.241	56.395	10.831	1.00 16.49
	ATOM	5621	OH2 TIP .	31	31.026	90.281	21.603	1.00 13.40
	MOTA	5622	OH2 TIP	32	16.272	85.213	27.168	1.00 31.73
10	MOTA	5623	OH2 TIP	33	34, 623	80.209	20.638	1.00 22.53
•	ATOM	5624	OH2 TIP	34	23.509	83.346	25.930	1.00 26.25
	ATOM	5625	OH2 TIP	. 35	68.471	35.753	-6.941	1.00 31.74
	ATOM	5626	OH2 TIP	36	42.708	91.595	-1.200	1.00 30.13
	MOTA	5627	OH2 TIP	37 .	73.882	57.001	9.723	1.00 .30.46
15	ATOM	5628	OH2 TIP	38	19.201	109.504	8.536	1.00 27.81
	ATOM	5629	OH2 TIP	39	66.027	53.748	25.075	1.00 23.62
	ATOM	5630	OH2 TIP	40	32.828	76.455	3.143	1.00 18.78
	ATOM	5631	OH2 TIP	41	31.297	75.533	-5.044	1.00 34.74
	MOTA	5632	OH2 TIP	42	46.752	86.115	9.500	1.00 41.15
20	MOTA	5633	OH2 TIP	43	45.965	90.475	9.941	1.00 19.78
	ATOM	5634	OH2 TIP	44	84.824	40.900	6.762	1.00 26.00
	MOTA	5635	OH2 TIP	45	88.709	40.949	11.546	1.00 24.12
	MOTA	·5636	OH2 TIP	46	33.051	73.353	10.148	1.00 34.00
	MOTA	5637	OH2 TIP	47	11.488	88.500	10.474	1.00 25.91
25	MOTA	5638	OH2 TIP	48 .	35.424	94.037	2.827	1.00 22.82
	MOTA	5639	OH2 TIP	49	73.417	40.151	1.138	1.00 33.97
	MOTA	5640	OH2 TIP	50	64.215	49.505	11.135	1.00 29.96
	MOTA	5641	OH2 TIP	51	35.946	77.916	5.004	1.00 22.91
	ATOM	5642	OH2 TIP	52	19.095	111.400	18.136	1.00 32.18
30	MOTA	5643	OH2 TIP	53	87.512	32.734	22.035	1.00 30.17
•	ATOM	5644	OH2 TIP	54	77.551	47.032	6.411	1.00 26.58
	MOTA	5645	OH2 TIP	55	86.637	41.109	3.619	
	ATOM	5646	OH2 TIP	56	58.706	37.981	-1.600	
	ATOM	5647	OH2 TIP	57	44.991	1 91.904	1.544	
. 35	ATOM	5648	OH2 TIP	. 58	82.87	1 58.902	12.437	1.00 29.62

	ATOM	5649	OH2 TIP	59	62.486	37.207	30.060	1.00	27.58
•	ATOM ·	5650	OH2 TIP	60	32.219	106.679	11.372	1.00	35.07
	MOTA	5651	OH2 TIP	61	68.981	58.634	30.748	1.00	27.70
	ATOM	5652	OH2 TIP	62	80.283	44.331	8.715	1.00	20.83
5	ATOM	5653	OH2 TIP	63	25.093	71.081	5.643	1.00	31.03
	ATOM	5654	OH2 TIP	64	38.840	87.644	18.843	1.00	32.58
	ATOM	5655	OH2 TIP	65 _.	35.643	97.747	-3.291	1.00	33.06
	ATOM	5656	OH2 TIP	66	28.484	90.260	29.530	1.00	38.62
	MOTA	5657	OH2 TIP	67	32.057	. 83.314	26.983	1.00	26.10
10	ATOM	5658	OH2 TIP	68	40.728	81.620	21.277	1.00	28.96
	ATOM	5659	OH2 TIP	69	83.110	48.185	-6.280	1.00	36.25
	MOTA	5660	OH2 TIP	70	13.308	79.186	19.324	1.00	27.35
	ATOM	5661	OH2 TIP	71	75.121	65.908	23.710	1.00	33.33
	ATOM	5662	OH2 TIP	72	72.885	49.529	31.358	1.00	43.43
15	ATOM	5663	OH2 TIP	73	90.409	43.863	22.223	1.00	35.52
	ATOM	5664	OH2 TIP	74	68.960	27.956	6.246	1.00	29.54
	ATOM	5665	OH2 TIP	75	68.759	24.978	13.691	1.00	36.46
	MOTA	5666	OH2 TIP	76	80.865	28.042	28.894	1.00	22.81
	MOTA	5667	OH2 TIP	77	83.513	20.534	2.136	1.00	44.57
20	MOTA	5668	OH2 TIP	78	33.991	88.631	-1.759 ·	1.00	47.18
	ATOM	5669	OH2 TIP	79	31.009	90.742	-1.589	1.00	35.71
	ATOM	5670	OH2 TIP	80	34.056	73.695	12.888	1.00	40.61
	MOTA	5671	OH2 TIP	81	71.030	59.790	1.571	1.00	34.14
	MOTA	5672	OH2 TIP	82	45.548	95.239	15.831	1.00	31.62
25	MOTA	5673	OH2 TIP	83	25.823	76.105	11.243	1.00	25.69
	MOTA	5674	OH2 TIP	84	75.453	38.146	30.507	1.00	25.25
	MOTA	5675	OH2 TIP	85 [*]	56.540	32.057	24.557	1.00	40.19
•	ATOM	5676	OH2 TIP	86	68.921	53.407	27.143	1.00	32.24
	ATOM	567 7	OH2 TIP	87	48.823	99.292	13.844	1.00	48.14
30	MOTA	5678	OH2 TIP	88	66.603	27.914	24.871	1.00	24.07
	MOTA	5679	OH2 TIP	89	72.553	25.024	4.480	1.00	37.79
	MOTA	5680	OH2 TIP	90	74.805	44.624	26.080	1.00	24.08
	MOTA	5681	OH2 TIP	91	82.314	60.516	10.339	1.00	28.44
	ATOM	5682	OH2 TIP	92	41.009	72.787	-2.680	1.00	49.99
35	MOTA	5683	OH2 TIP	93	75.218	36.521	28.025	1.00	21.73

ATOM	5684	OH2 TIP	94	58.786	33.514	-1.584	1.00 46.12
ATOM	5685	OH2 TIP	95	59.443	56.186	13.092	1.00 24.57
MOTA	5686	OH2 TIP .	96	44.571	79.740	17.158	1.00 33.72
ATOM	5687	OH2 TIP	97	36.543	97.946 .	22.228	1.00 20.11
MOTA	5688	OH2 TIP	98	42.102	91.284 ·	4.898	1.00 22.27
MOTA	5689	OH2 TIP	99	83.993	26.068	16.812	1.00 39.48
MOTA	5690	OH2 TIP	100	71.425	22.395	31.294	1.00 42.78
MOTA	5691	OH2 TIP	101	41.521	86.237	20.453	1.00 36.59
MOTA	5692	OH2 TIP	102	77.290	21.465	18.797	1.00 39.54
ATOM ,	5693	OH2 TIP	103	34.574	71.613	8.514	1.00 40.98
ATOM	5694	OH2 TIP	104	80.216	58.145	30.951	1.00 31.65
MOTA	5695	OH2 TIP	105	51.953	83.113	-1.215	1.00 34.53
ATOM	5696	OH2 TIP	106	78.065	52.209	26.693	1.00 31.02
MOTA	5697	OH2 TIP	107	68.221	20.544	13.056	1.00 29.84
ATOM	5698	OH2 TIP	108	9.340	73.178	-1.320	1.00 27.34
ATOM	5699	OH2 TIP	109	82.865	28.096	7.563	1.00 24.08
MOTA	5700	OH2 TIP	110	51.681	22.615	23.853	1.00 42.57
ATOM	5701	OH2 TIP	111	80.577	21.841	24.237	1.00 38.89
MOTA	5702	OH2 TIP	112	29.043	102.944	3.861	1.00 36.35
MOTA	5703	OH2 TIP	113	34.227	97.988	29.010	1.00 29.76
ATOM	5704	OH2 TIP	114	40.735	90.064	18.442	1.00 46.42
MOTA	5705	OH2 TIP	115	25.295	100.974	13.456	1.00 25.31
MOTA	5706	OH2 TIP	116	75.441	52.065	2.449	1:00 19.42
MOTA	5707	OH2 TIP	117	74.070	56.553	-0.631	1.00 47.18
ATOM	5708	OH2 TIP	118	65.566	64.590	9.062	1.00 44.16
ATOM	5709	OH2 TIP	119	60.666	43.201	3.854	1.00 34.57
MOTA	5710	OH2 TIP	120	76.120	45.123	29.617	1.00 36.08
ATOM	5711	OH2 TIP	121	54.142	51.739	14.688	1.00 31.52
MOTA	5712	OH2 TIP	122	39.719	105.971	10.102	1.00 27.01
ATOM	5713	OH2 TIP	123	85.171	44.498	7.479	1.00 31.29
MOTA	5714	OH2 TIP	. 124	86.210	29.970	-11.184	1.00 29.65
MOTA	5715	OH2 TIP	125	72.634	31.654	-0.249	1.00 25.24
ATOM	5716	OH2 TIP	126	16.147	70.198	22.206	1.00 28.88
ATOM	5717	OH2 TIP	127	37.233	69.031	17.117	1.00 39.61
ATOM	5718	OH2 TIP	128	35.202	98.368	26.457	1.00 23.25
	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	ATOM 5685 ATOM 5686 ATOM 5687 ATOM 5688 ATOM 5689 ATOM 5690 ATOM 5691 ATOM 5692 ATOM 5693 ATOM 5693 ATOM 5695 ATOM 5695 ATOM 5696 ATOM 5697 ATOM 5698 ATOM 5699 ATOM 5700 ATOM 5701 ATOM 5702 ATOM 5702 ATOM 5703 ATOM 5704 ATOM 5705 ATOM 5706 ATOM 5707 ATOM 5708 ATOM 5708 ATOM 5709 ATOM 5710 ATOM 5711 ATOM 5712 ATOM 5713 ATOM 5715 ATOM 5715 ATOM 5715 ATOM 5715 ATOM 5716 ATOM 5715 ATOM 5716 ATOM 5715 ATOM 5715	ATOM 5685 OH2 TIP ATOM 5686 OH2 TIP ATOM 5687 OH2 TIP ATOM 5688 OH2 TIP ATOM 5689 OH2 TIP ATOM 5690 OH2 TIP ATOM 5691 OH2 TIP ATOM 5692 OH2 TIP ATOM 5693 OH2 TIP ATOM 5694 OH2 TIP ATOM 5696 OH2 TIP ATOM 5698 OH2 TIP ATOM 5698 OH2 TIP ATOM 5700 OH2 TIP ATOM 5701 OH2 TIP ATOM 5703 OH2 TIP ATOM 5704 OH2 TIP ATOM 5705 OH2 TIP ATOM 5706 OH2 TIP ATOM 5709 </td <td>ATOM 5685 OH2 TIP 95 ATOM 5686 OH2 TIP 96 ATOM 5687 OH2 TIP 97 ATOM 5688 OH2 TIP 98 ATOM 5689 OH2 TIP 99 ATOM 5689 OH2 TIP 100 ATOM 5690 OH2 TIP 100 ATOM 5691 OH2 TIP 102 ATOM 5693 OH2 TIP 103 ATOM 5693 OH2 TIP 103 ATOM 5694 OH2 TIP 105 ATOM 5695 OH2 TIP 105 ATOM 5696 OH2 TIP 106 ATOM 5697 OH2 TIP 107 ATOM 5698 OH2 TIP 108 ATOM 5699 OH2 TIP 108 ATOM 5699 OH2 TIP 109 ATOM 5700 OH2 TIP 109 ATOM 5701 OH2 TIP 111 ATOM 5702 OH2 TIP 111 ATOM 5703 OH2 TIP 111 ATOM 5704 OH2 TIP 111 ATOM 5705 OH2 TIP 113 ATOM 5706 OH2 TIP 114 ATOM 5706 OH2 TIP 116 ATOM 5707 OH2 TIP 116 ATOM 5708 OH2 TIP 117 ATOM 5708 OH2 TIP 118 ATOM 5709 OH2 TIP 119 ATOM 5709 OH2 TIP 119 ATOM 5700 OH2 TIP 110 ATOM 5701 OH2 TIP 111 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 121 ATOM 5701 OH2 TIP 122 ATOM 5710 OH2 TIP 122 ATOM 5711 OH2 TIP 122 ATOM 5711 OH2 TIP 122 ATOM 5713 OH2 TIP 122 ATOM 5714 OH2 TIP 123 ATOM 5715 OH2 TIP 124 ATOM 5716 OH2 TIP 124 ATOM 5716 OH2 TIP 125 ATOM 5717 OH2 TIP 126 ATOM 5718 OH2 TIP 121 ATOM 5719 OH2 TIP 122 ATOM 5711 OH2 TIP 123 ATOM 5711 OH2 TIP 124 ATOM 5712 OH2 TIP 125 ATOM 5713 OH2 TIP 126 ATOM 5716 OH2 TIP 126 ATOM 5716 OH2 TIP 126</td> <td>ATOM 5685 OH2 TIP 95 59.443 ATOM 5686 OH2 TIP 96 44.571 ATOM 5687 OH2 TIP 97 36.543 ATOM 5688 OH2 TIP 98 42.102 ATOM 5689 OH2 TIP 99 83.993 ATOM 5690 OH2 TIP 100 71.425 ATOM 5691 OH2 TIP 101 41.521 ATOM 5692 OH2 TIP 102 77.290 ATOM 5693 OH2 TIP 103 34.574 ATOM 5694 OH2 TIP 104 80.216 ATOM 5695 OH2 TIP 105 51.953 ATOM 5696 OH2 TIP 106 78.065 ATOM 5696 OH2 TIP 107 68.221 ATOM 5698 OH2 TIP 108 9.340 ATOM 5699 OH2 TIP 109 82.865 ATOM 5700 OH2 TIP 110 51.681 ATOM 5701 OH2 TIP 111 80.577 ATOM 5702 OH2 TIP 112 29.043 ATOM 5703 OH2 TIP 114 40.735 ATOM 5706 OH2 TIP 115 25.295 ATOM 5706 OH2 TIP 116 75.441 ATOM 5707 OH2 TIP 117 74.070 ATOM 5708 OH2 TIP 118 65.566 ATOM 5709 OH2 TIP 119 60.666 ATOM 5701 OH2 TIP 110 76.120 ATOM 5701 OH2 TIP 120 76.120 ATOM 5701 OH2 TIP 121 39.719 ATOM 5702 OH2 TIP 122 39.719 ATOM 5703 OH2 TIP 123 85.171 ATOM 5704 OH2 TIP 124 86.210 ATOM 5711 OH2 TIP 124 86.210 ATOM 5713 OH2 TIP 124 86.210 ATOM 5713 OH2 TIP 125 72.634 ATOM 5715 OH2 TIP 125 72.634 ATOM 5716 OH2 TIP 127 37.233</td> <td>ATOM 5685 OH2 TIP 95 59.443 56.186 ATOM 5686 OH2 TIP 96 44.571 79.740 ATOM 5687 OH2 TIP 97 36.543 97.946 ATOM 5688 OH2 TIP 98 42.102 91.284 ATOM 5689 OH2 TIP 99 83.993 26.068 ATOM 5690 OH2 TIP 100 71.425 22.395 ATOM 5691 OH2 TIP 101 41.521 86.237 ATOM 5692 OH2 TIP 102 77.290 21.465 ATOM 5693 OH2 TIP 103 34.574 71.613 ATOM 5694 OH2 TIP 103 34.574 71.613 ATOM 5695 OH2 TIP 104 80.216 58.145 ATOM 5696 OH2 TIP 105 51.953 83.113 ATOM 5696 OH2 TIP 106 78.065 52.209 ATOM 5697 OH2 TIP 107 68.221 20.544 ATOM 5698 OH2 TIP 108 9.340 73.178 ATOM 5699 OH2 TIP 109 82.865 28.096 ATOM 5700 OH2 TIP 110 51.681 22.615 ATOM 5701 OH2 TIP 111 80.577 21.841 ATOM 5702 OH2 TIP 112 29.043 102.944 ATOM 5703 OH2 TIP 113 34.227 97.988 ATOM 5704 OH2 TIP 114 40.735 90.064 ATOM 5705 OH2 TIP 115 25.295 100.974 ATOM 5707 OH2 TIP 116 75.441 52.065 ATOM 5709 OH2 TIP 117 74.070 56.553 ATOM 5709 OH2 TIP 118 65.566 64.590 ATOM 5710 OH2 TIP 119 60.666 43.201 ATOM 5710 OH2 TIP 119 60.666 43.201 ATOM 5710 OH2 TIP 120 76.120 45.123 ATOM 5710 OH2 TIP 121 54.142 51.739 ATOM 5711 OH2 TIP 122 39.719 105.971 ATOM 5712 OH2 TIP 123 85.171 44.498 ATOM 5713 OH2 TIP 124 86.210 29.970 ATOM 5714 OH2 TIP 124 86.210 29.970 ATOM 5715 OH2 TIP 125 72.634 31.654 ATOM 5716 OH2 TIP 126 16.147 70.198 ATOM 5716 OH2 TIP 127 37.231 69.031</td> <td>ATOM 5685 OH2 TIP 95 59.443 \$6.186 13.092 ATOM 5686 OH2 TIP 96 44.571 79.740 17.158 ATOM 5687 OH2 TIP 97 36.543 97.946 22.228 ATOM 5688 OH2 TIP 98 42.102 91.284 4.898 ATOM 5689 OH2 TIP 99 83.993 26.068 16.812 ATOM 5690 OH2 TIP 100 71.425 22.395 31.294 ATOM 5692 OH2 TIP 101 41.521 86.237 20.453 ATOM 5693 OH2 TIP 103 34.574 71.613 8.514 ATOM 5694 OH2 TIP 104 80.216 58.145 30.951 ATOM 5695 OH2 TIP 105 51.953 83.113 -1.215 ATOM 5696 OH2 TIP 106 78.065 52.209 26.693 ATOM 5697 OH2 TIP 107 68.221 20.544 13.056 ATOM 5698 OH2 TIP 108 9.340 73.178 -1.320 ATOM 5699 OH2 TIP 109 82.865 28.096 7.563 ATOM 5700 OH2 TIP 110 51.681 22.615 23.853 ATOM 5700 OH2 TIP 111 80.577 21.841 24.237 ATOM 5700 OH2 TIP 112 29.043 102.944 3.861 ATOM 5700 OH2 TIP 114 40.735 90.064 18.442 ATOM 5700 OH2 TIP 115 25.295 100.974 13.456 ATOM 5700 OH2 TIP 116 75.441 52.065 2.449 ATOM 5700 OH2 TIP 117 74.070 56.553 -0.631 ATOM 5700 OH2 TIP 118 65.566 64.590 9.062 ATOM 5700 OH2 TIP 119 60.666 43.201 3.854 ATOM 5700 OH2 TIP 119 60.666 43.201 3.854 ATOM 5701 OH2 TIP 119 60.666 43.201 3.854 ATOM 5702 OH2 TIP 119 60.666 43.201 3.854 ATOM 5703 OH2 TIP 119 60.666 43.201 3.854 ATOM 5704 OH2 TIP 119 60.666 43.201 3.854 ATOM 5709 OH2 TIP 120 76.120 45.123 29.617 ATOM 5710 OH2 TIP 121 54.142 51.739 14.688 ATOM 5710 OH2 TIP 122 39.719 105.971 10.102 ATOM 5711 OH2 TIP 123 85.171 44.498 7.479 ATOM 5713 OH2 TIP 124 86.210 29.970 -11.1.84 ATOM 5714 OH2 TIP 124 86.210 29.970 -11.1.84 ATOM 5715 OH2 TIP 125 72.634 31.654 -0.249 ATOM 5716 OH2 TIP 126 16.147 70.198 22.206</td>	ATOM 5685 OH2 TIP 95 ATOM 5686 OH2 TIP 96 ATOM 5687 OH2 TIP 97 ATOM 5688 OH2 TIP 98 ATOM 5689 OH2 TIP 99 ATOM 5689 OH2 TIP 100 ATOM 5690 OH2 TIP 100 ATOM 5691 OH2 TIP 102 ATOM 5693 OH2 TIP 103 ATOM 5693 OH2 TIP 103 ATOM 5694 OH2 TIP 105 ATOM 5695 OH2 TIP 105 ATOM 5696 OH2 TIP 106 ATOM 5697 OH2 TIP 107 ATOM 5698 OH2 TIP 108 ATOM 5699 OH2 TIP 108 ATOM 5699 OH2 TIP 109 ATOM 5700 OH2 TIP 109 ATOM 5701 OH2 TIP 111 ATOM 5702 OH2 TIP 111 ATOM 5703 OH2 TIP 111 ATOM 5704 OH2 TIP 111 ATOM 5705 OH2 TIP 113 ATOM 5706 OH2 TIP 114 ATOM 5706 OH2 TIP 116 ATOM 5707 OH2 TIP 116 ATOM 5708 OH2 TIP 117 ATOM 5708 OH2 TIP 118 ATOM 5709 OH2 TIP 119 ATOM 5709 OH2 TIP 119 ATOM 5700 OH2 TIP 110 ATOM 5701 OH2 TIP 111 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 112 ATOM 5701 OH2 TIP 121 ATOM 5701 OH2 TIP 122 ATOM 5710 OH2 TIP 122 ATOM 5711 OH2 TIP 122 ATOM 5711 OH2 TIP 122 ATOM 5713 OH2 TIP 122 ATOM 5714 OH2 TIP 123 ATOM 5715 OH2 TIP 124 ATOM 5716 OH2 TIP 124 ATOM 5716 OH2 TIP 125 ATOM 5717 OH2 TIP 126 ATOM 5718 OH2 TIP 121 ATOM 5719 OH2 TIP 122 ATOM 5711 OH2 TIP 123 ATOM 5711 OH2 TIP 124 ATOM 5712 OH2 TIP 125 ATOM 5713 OH2 TIP 126 ATOM 5716 OH2 TIP 126 ATOM 5716 OH2 TIP 126	ATOM 5685 OH2 TIP 95 59.443 ATOM 5686 OH2 TIP 96 44.571 ATOM 5687 OH2 TIP 97 36.543 ATOM 5688 OH2 TIP 98 42.102 ATOM 5689 OH2 TIP 99 83.993 ATOM 5690 OH2 TIP 100 71.425 ATOM 5691 OH2 TIP 101 41.521 ATOM 5692 OH2 TIP 102 77.290 ATOM 5693 OH2 TIP 103 34.574 ATOM 5694 OH2 TIP 104 80.216 ATOM 5695 OH2 TIP 105 51.953 ATOM 5696 OH2 TIP 106 78.065 ATOM 5696 OH2 TIP 107 68.221 ATOM 5698 OH2 TIP 108 9.340 ATOM 5699 OH2 TIP 109 82.865 ATOM 5700 OH2 TIP 110 51.681 ATOM 5701 OH2 TIP 111 80.577 ATOM 5702 OH2 TIP 112 29.043 ATOM 5703 OH2 TIP 114 40.735 ATOM 5706 OH2 TIP 115 25.295 ATOM 5706 OH2 TIP 116 75.441 ATOM 5707 OH2 TIP 117 74.070 ATOM 5708 OH2 TIP 118 65.566 ATOM 5709 OH2 TIP 119 60.666 ATOM 5701 OH2 TIP 110 76.120 ATOM 5701 OH2 TIP 120 76.120 ATOM 5701 OH2 TIP 121 39.719 ATOM 5702 OH2 TIP 122 39.719 ATOM 5703 OH2 TIP 123 85.171 ATOM 5704 OH2 TIP 124 86.210 ATOM 5711 OH2 TIP 124 86.210 ATOM 5713 OH2 TIP 124 86.210 ATOM 5713 OH2 TIP 125 72.634 ATOM 5715 OH2 TIP 125 72.634 ATOM 5716 OH2 TIP 127 37.233	ATOM 5685 OH2 TIP 95 59.443 56.186 ATOM 5686 OH2 TIP 96 44.571 79.740 ATOM 5687 OH2 TIP 97 36.543 97.946 ATOM 5688 OH2 TIP 98 42.102 91.284 ATOM 5689 OH2 TIP 99 83.993 26.068 ATOM 5690 OH2 TIP 100 71.425 22.395 ATOM 5691 OH2 TIP 101 41.521 86.237 ATOM 5692 OH2 TIP 102 77.290 21.465 ATOM 5693 OH2 TIP 103 34.574 71.613 ATOM 5694 OH2 TIP 103 34.574 71.613 ATOM 5695 OH2 TIP 104 80.216 58.145 ATOM 5696 OH2 TIP 105 51.953 83.113 ATOM 5696 OH2 TIP 106 78.065 52.209 ATOM 5697 OH2 TIP 107 68.221 20.544 ATOM 5698 OH2 TIP 108 9.340 73.178 ATOM 5699 OH2 TIP 109 82.865 28.096 ATOM 5700 OH2 TIP 110 51.681 22.615 ATOM 5701 OH2 TIP 111 80.577 21.841 ATOM 5702 OH2 TIP 112 29.043 102.944 ATOM 5703 OH2 TIP 113 34.227 97.988 ATOM 5704 OH2 TIP 114 40.735 90.064 ATOM 5705 OH2 TIP 115 25.295 100.974 ATOM 5707 OH2 TIP 116 75.441 52.065 ATOM 5709 OH2 TIP 117 74.070 56.553 ATOM 5709 OH2 TIP 118 65.566 64.590 ATOM 5710 OH2 TIP 119 60.666 43.201 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	MOTA	5719	OH2	TIP	129	101.610	39.762	-20.072	1.00	30.45
	MOTA	5720	OH2	TIP	130	62.699	33.014	-2.726	1.00	42.68
	MOTA	5721	OH2	TIP	131	66.836	50.243	30.662	1.00	39.68
	ATOM	5722	OH2	TIP	132	5.358	93.633	. 5.849	1.00	48.29
5	ATOM	5723°	OH2	TIP	133	87.786	24.130	-16.104	1.00	39.99
•	ATOM	5724	OH2	TIP	134 .	42.301	75.221	8.757	1.00	42.10
	ATOM	5725	OH2	TIP	135	78.036	44.723	-10.662	1.00	37.65
	MOTA	5726	ОН2	TIP	136	38.073	90.012	21.232	1.00	23.10
	MOTA	5727	OH2	TIP	1.37	24.581	92.415	-2.442	1.00	37.05
10	MOTA	5728	OH2	TIP.	138	12.396	106.041	18.053	1.00	43.25
•	ATOM	5729	OH2	TIP	139	77.977	34.593	3.036	1.00	25.44
	MOTA	· 5730	OH2	TIP	140	40.297	92.891	-1.662	1.00	40.79
	ATOM	5,731	OH2	TIP	141	35.031	85.843	-0.290	1.00	30.75
	MOTA	5732	OH2	TIP	142	.78.177	49.267	4.406	1.00	44.08
15	MOTA	5733	OH2	TIP.	143	44.684	85.363	-13.653	1.00	42.96
	ATOM	5734	OH2	TIP	144	16.523	68.716	10.379	1.00	44.38
	ATOM	5735	OH2	ΤΊΡ	145	37.171	84.228	20.730	1.00	37.73
	ATOM	5736	OH2	TIP	146	84.109	34.734	25.222	1.00	28.75
	MOTA	5737	OH2	TIP	147	13.573	65.829	5.292	1.00	41.32
20	MOTA	5738	OH2	TIP	148	87.775	51.477	19.308	1.00	33.04
•	ATOM	5739	OH2	TIP	149	61.055	46.851	29.860	1.00	38.86
	MOTA	5740	OH2	TIP	150	30.709	93.775	30.547	1.00	35.96
	ATOM	5741	OH2	TIP	151	16.687	95.444	4.127	1:00	34.28
	ATOM	5742	OH2	TIP	152	20.727	95.654	3.238	1.00	38.20
25	ATOM	5743	OH2	TIP	153	77.522	26.578	-16.506	1.00	34.79
	MOTA	5744	OH2	TIP	. 154	17.542	77.986	26.146	1.00	40.07
	MOTA	5745	OH2	TIP	155	63.161	38.672	-5.820	1.00	54.97
	MOTA	5746	OH2	TIP	156	74.192	34.524	35.857	1.00	57.51
	MOTA	5747	OH2	TIP	157	21.552	99.456	10.491	1.00	27.88
30	MOTA .	5748	OH2	TIP	158	83.085	24.564	22.892	1.00	31.49
	MOTA	5749	OH2	TIP	159	47.798	39.263	-2.076	1.00	54.69
	ATOM	5750	OH2	TIP	160	88.099	51.183	23.984	1.00	35.12
	MOTA	5751	OH2	TIP	161	24.423	92.769	30.535	1.00	38.45
	ATOM	5752	OH2	TIP	162	63.166	20.190	11.461	1.00	46.78
35	ATOM	5753	OH2	TIP	163	59.098	44.329	5.827	1.00	33.01

	ATOM	5754	OH2 TIP	164	13.507	107.912	20.781	1.00 3	5.72
•	ATOM	5755	OH2 TIP	165	83.412	61.086	22.636	1.00 3	5.01
	ATOM	5756	OH2 TIP	166	49.112	73.913	6.534	1.00 6	6.27
	ATOM	5757	OH2 TIP	167	91.394	32.212 .	10.337	1.00 5	0.39
5	MOTA	5758	OH2 TIP	168	6.449	94.287	26.888	1.00 4	7.63
	ATOM	5759	OH2 TIP	169	76.464	68.219	23.721	1.00 5	3.79
	ATOM	5760	OH2 TIP	170	22.808	74.862	19.059	1.00 3	33.21
	ATOM	5761	OH2 TIP	171	48.317	80.149	7.342	1.00 2	27.26
	ATOM	5762	OH2 TIP	172	41.162	85.237	-16.033	1.00 3	39.98
10	MOTA	5763	OH2 TIP	173	51.407	31.394	15.649	1.00 4	12.59
	ATOM	5764	OH2 TIP	174	22.955	60.844	22.421 .	1.00 3	38.82
	ATOM	5765	OH2 TIP	175	28.394	98.779	1.827	1.00 4	11.53
	ATOM	5766	OH2 TIP	176 ·	69.684	65.594	24.524	1.00	14.96
	ATOM	5767	OH2 TIP	177	43.200	93.280	3.459	1.00	34.13
15	ATOM	5768	OH2 TIP	178	17.756	90.119	27.355	1.00	45.97
	MOTA	5769	OH2 TIP	179	105.475	.35.722	3.208	1.00	46.41
	MOTA	5770	OH2 TIP	180	18.511	69.070	13.131	1.00	44.83
	ATOM	5771	OH2 TIP	181	34.777	83.786	27.054	1.00	49.09
	MOTA	5772	OH2 TIP	182	76.901	25.642	31.034	1.00	47.31
20	MOTA	5773	OH2 TIP	183	48.876	35.979	8.482	1.00	32.37
	ATOM	5774	OH2 TIP	184	25.637	99.645	26.739	1.00	45.36
•	MOTA	5775	OH2 TIP	- 185	93.103	36.239	0.414	1.00	33.77
	MOTA	5776	OH2 TIP	186	71.600	55.767	30.268	1.00	32.79
	ATOM	5777	OH2 TIP	187	15.541	76.607	2.456	1.00	41.98
25	ATOM	5778	OH2 TIP	188	41.719	74.503	14.650	1.00	51.88
	ATOM	5779	OH2 TIP	189	75.164	69.545	21.068	1.00	52.07
	MOTA	5780	OH2 TIP	190	74.872	2 39.797	-2.637	. 1.00	41.24
	MOTA	5781	OH2 TIP	191	22.684	97.520	3.087	1.00	37.30
	ATOM	5782	OH2 TIP	192	25.46	7 107.654	1.749	1.00	41.11
30	MOTA	5783	OH2 TIP	193	69.28	2 51.934	2.697	1.00	41.69
	MOTA	5784	OH2 TIP	194	38.99	4 107.268	27.347	1.00	37.35
	MOTA	5785	OH2 TIP	195	63.09	2 51.837	28.741	1.00	38.92
•	ATOM	5786	OH2 TIP	196	11.48	7 77.282	0.147	1.00	36.21
	ATOM	5787	OH2 TIP	197	36.15	0 94.786	-15.531	1.00	39.60
35	MOTA	5788	OH2 TIP	198	82.36	0 44.024	21.173	1.00	36.55

	ATOM	5789	OH2	TIP	199	35.092	94.097	23.903	1.00	32.06
	ATOM	5790	ОН2	TIP	200	63.021	70.590	15.903	1.00	56.60
	MOTA	5791	ОН2	TIP	201	49.283	43.418	9.849	1.00	47.58
	ATOM	5792	OH2	TIP .	202	36.906	100.577	.21.840	1.00	40.78
5	ATOM	5793	OH2	TIP	203	76.551	63.953	25.972	1.00	35.46
	ATOM	5794	OH2	TIP	204	87.842	55.120	11.824	1.00	29.94
	ATOM	5795	OH2	TIP	205	36.937	66.014	-8.244	1.00	41.61
	ATOM	5796	OH2	TIP	206	82.257	40.382	21.175	1.00	36.08
	ATOM	5797	OH2	TIP	207	75.418	44.375	-1.993	1.00	40.61
10	ATOM	5798	OH2	TIP	208	8.151	69.166	16.710	1.00	44.90
	ATOM	5799	OH2	TIP	209	83.811	57.022	19.559	1.00	23.75
	ATOM	5800	OH2	TIP	210	89.732	38.502	10.624	1.00	45.38
	ATOM	5801	OH2	TIP	211 .	57.995	53.900	13.742	1.00	45.45
	ATOM	5802	OH2	TIP	212	41.221	100.360	-7.718	1.00	49.06
15	ATOM	5803	OH2	TIP	213	72.092	37.629	32.475	1.00	61.51
	ATOM	5804	OH2	TIP	214	37.776	74.115	23.513	1.00	53.60
	ATOM	5805	OH2	TIP	215	95.633	49.033	19.239	1.00	39.53
4	ATOM	5806	OH2	TIP	216	15.800	72.932	22.618	1.00	47.69
	MOTA	5807	OH2	TIP	217	63.637	26.806	29.999	1.00	42.46
20	ATOM	5808	OH2	TIP	218	48.894	66.556	-18.212	1.00	40.87
	MOTA	5809	OH2	TIP	219	76.997	21.646	4.056	1.00	37.21
	ATOM	5810	OH2	TIP	220	86.518	26.866	20.224	1.00	45.02
	MOTA	5811	· OH2	TIP	221	44.243	.76.229	10.420	1.00	38.37
	MOTA	5812	OH2	TIP	222	25.182	88.366	-6.548	1.00	37.81
25	MOTA	5813	OH2	TIP	223	99.608	46.589	-2.471	1.00	52.75
	MOTA	5814	OH2	TIP	224	64.098	59.015	25.988	1.00	34.05
	MOTA	5815	OH2	TIP	225	49.905	102.416	19.684	1.00	44.14
	MOTA	5816	OH2	TIP	226	91.136	36.314	11.446	1.00	47.05
	MOTA	5817	OH2	TIP	227	81.387	55.146	27.778	1.00	47.39
30	ATOM	5818	OH2	TIP	228	60.811	69.016	15.894	1.00	48.74
	MOTA	5819	OH2	TIP	229	60.946	61.261	26.309	1.00	54.59
	ATOM	5820	OH2	TIP	230	33.525	74.075	4.130	1.00	51.65
	ATOM	5821	OH2	TIP	231	85.430	32.491	-10.569	1.00	31.56
	ATOM	5822	OH2	TIP	232	12.280	91.312	-6.338	1.00	37.69
35	ATOM	5823	OH2	TIP	233	29.661	83.836	-4.637	1.00	33.62

	ATOM	5824	OH2 TIP	234	. 68.894	24.672	2.939	1.00 31.68
	ATOM	5825	OH2 TIP	235	84.378	21.827	27.009	1.00 38.47
	ATOM	5826	OH2 TIP	236	61.770	41.536	29.780	1.00 28.87
	MOTA	5827	OH2 TIP	237	22.526	69.316	12:108	1.00 56.68
5	ATOM	5828	OH2 TIP	238	72.573	40.681	-4.565	1.00 41.36
	ATOM	5829	OH2 TIP	239	64.589	45.566	4.403	1.00 21.60
	ATOM	5830	OH2 TIP	240	39.921	76.650 -	25.549	1.00 42.96
	ATOM	5831	OH2 TIP	241	37.402	83.028	26.817	1.00 45.34
•	ATOM	5832	OH2 TIP	242	33.290	71.184	24.438	1.00 41.99
10	ATOM	5833	OH2 TIP	243	20.114	105.283	26.910	1.00 42.62
	ATOM	5834	OH2 TIP	244	72.442	42.860	29.082	1.00 42.21
	ATOM	5835	OH2 TIP	245	13.992	82.149	1.241	1.00 38.85
	ATOM	5836	OH2 TIP	246	41.909	97.922	17.548	1.00 41.20
	ATOM	5837	OH2 TIP	247	72.472	45.709	8.588	1.00 21.46
15	MOTA	5838	OH2 TIP	248	70.421	54.773	-0.661	1.00 43.75
	ATOM	5839	OH2 TIP	249	67.143	38.463	0.215	1.00 36.80
	ATOM	5840	OH2 TIP	250	87.976	55.453	18.319	1.00 28.56
	MOTA	5841	OH2 TIP	251	69.999	46.346	31.247	1.00 39.70
	ATOM	5842	OH2 TIP	252	54.539	50.747	4.830	1.00 37.48
20	ATOM	5843	OH2 TIP	253	21.028	80.517	26.853	1.00 44.29
	MOTA	5844	OH2 TIP	254	18.684	98.982	25.594	1.00 37.90
	MOTA	5845	OH2 TIP	255	70.229	34.803	-1.368	1.00 60.61
	ATOM	5846	OH2 TIP	256	87.106	48.869	19.010	1.00 32.54
	ATOM	5847	OH2 TIP	257	47.420	88.249	7.951	1.00 35.67
25	ATOM	5848	OH2 TIP	258	21.063	3 115.438	17.316	1.00 35.89
	MOTA	5849	OH2 TIP	259	24.427	110.948	2.222	1.00 34.03
	ATOM	5850	OH2 TIP	. 260	52.830	46.305	6.084	1.00 39.87
	ATOM	5851	OH2 TIP	261	42.265	5 94.805	19.620	1.00 24.07
	ATOM	5852	OH2 TIP	262	56.05	7 57.733	27.560	1.00 42.47
30	ATOM	5853	OH2 TIP	263	19.35	1 82.738	26.360	1.00 35.37
	ATOM	5854	OH2 TIP	264	23.14	4 73.194	30.688	1.00 47.32
	ATOM	5855	OH2 TIP	265	63.01	3 62.906	25.680	1.00 38.65
	ATOM	5856	OH2 TIP	266	41.85	9 70.029	-12.808	•
	ATOM	5857	OH2 TIP	267	41.04	7 94.499	-12.252	1.00 30.89
35	ATOM	5858	OH2 TIP	268	49.32	2 44.383	24.746	1.00 57.50

	ATOM	5859	OH2	TIP	269	14.345	83.254	27.072	1.00	47.73
	ATOM	5860	OH2	TIP	270	84.431	23.892	-19.636	1.00	50.82
	ATOM	5861	OH2	TIP	271	7.771	98.423	13.702	1.00	46.11
	ATOM	5862	OH2	TIP	272	13.603	76.350	2.466	1.00	47.00
5	ATOM	5863	OH2	TIP	273	43.175	41.193	4.583	1.00	40.21
	ATOM	5864	OH2	TIP	274	58.291	51.532	7.003	1.00	54.17
	ATOM	5865	OH2	TIP	275	51.325	90.886	14.219	1.00	42.67
	ATOM	5866	OH2	TIP	276	86.090	56 [.] .149	23.228	1.00	40.06
	ATOM	5867	ОН2	TIP	277	50.966	45.969	21.203	1.00	32.47
10	MOTA	5868	OH2	TIP	278	89.100	42.135	3.527	1.00	47.40
	ATOM	58 69	ОН2	TIP	279	17.273	95.041	1.168	1.00	43.83
	ATOM:	5870	OH2	TIP	280	58.673	98.407	-7.046	1.00	45.08
	ATOM	5871	OH2	TIP	281	78.163	17.076	4.589	1.00	46.28
	ATOM	5872	ОН2	TIP	282	101.345	35.952	7.650	1.00	41.44
15	ATOM	5873	OH2	TIP	283	58.562	28.216	31.037	1.00	37.19
	MOTA	5874	OH2	TIP	284	3.431	93.236	20.866	1.00	46.44
	ATOM	5875	OH2	TIP	285	46.206	100.458	11.278	1.00	42.03
	ATOM	5876	OH2	TIP	286	7.144	99.468	5.033	1.00	60.41
•	MOTA	5877	OH2	TIP	287	56.442	16.403	16.295	1.00	48.75
20	ATOM	5878	OH2	TIP	288	72.651	59.077	36.505	1.00	45.43
	MOTA	5879	OH2	TIP	289	15.525	86.890	-5.252	1.00	45.27
	MOTA	5880	OH2	TIP	290	52.750	75.991	4.087	1.00	52.62
	MOTA	5881	OH2	TIP	291	48.875	99.238	-12.260	1.00	44.59
	MOTA	5882	OH2	TIP	292	46.786	90.537	21.400	1.00	39.68
25	MOTA	5883	OH2	TIP	293	85.515	48.612	7.509	1.00	34.49
	MOTA	5884	OH2	TIP	294	7.945	73.643	11.102	1.00	42.36
	MOTA	5885	OH2	TIP	295	18.140	70.001	15.786	1.00	43.51
	ATOM	5886	OH2	TIP	296	54.034	38.692	-2.318	1.00	46.78
	ATOM	5887	OH2	TIP	297	58.790	38.984	30.000	1.00	42.56
30	ATOM	5888	OH2	TIP	298	53.117	25.322	21.425	1.00	48.65
	MOTA	5889	OH2	TIP	299	79.667	23.687	28.724	1.00	31.36
	ATOM	5890	OH2	TIP	300	65.052	55.747	26.794	1.00	43.24
	ATOM	5891	OH2	TIP	301	82.283	36.493	26.079	1.00	36.32
	MOTA	5892	OH2	TIP	302	27.538	89.554	-2.616	1.00	41.41
35	MOTA	5893	OH2	TIP	303	55.070	40.595	29.011	1.00	38.03

	ATOM	5894	он2 т	IP	304	101.938	39.946	-7.588	1.00 47.50
	MOTA	5895	онг т	IP	305	94.519	53.023	16.596	1.00 46.73
	ATOM	5896	он2 т	IР	306	4.609	98.144	17.159	1.00 47.55
	ATOM	5897	он2 т	IP	307	72.568	17727	20.484	1.00 43.07
5	ATOM	5898	OH2 T	IP	308	44.734	92.751	-18.906	1.00 41.46
	ATOM	5899	OH2 T	P	309	39.432	70.028	-8.496	1.00 43.09
	MOTA	5900	OH2 I	TIP	310	78.014	22.700	12.525	1.00 38.49
	ATOM	5901	OH2 I	rip	311	15.607	102.239	7.211	1.00 40.40
	MOTA	5902	OH2	rip	312	62.505	32.788	30.140	1.00 27.47
10	ATOM	5903	OH2	rip	313	16.926	100.528	24.125	1.00 42.11
	ATOM	5904	OH2 :	rip	314	88.342	39.723	21.124	1.00 27.74
	ATOM	5905	он'2 '	TIP	315 .	66.669	57.207	0.563	1.00 37.58
	ATOM	5906	OH2	TIP	316	59.985	92.952	-1.731	1.00 41.14
	ATOM	5907	OH2	TIP	317	75.200	40.815	31.050	1.00 46.78
15	ATOM	5908	OH2	TIP	318	89.890	31.775	17.421	1.00 43.01
	ATOM	5909	ОН2	TIP	319	36.404	68.064	5.905	1.00 56.47
	MOTA	5910	OH2	TIP	320	84.306	.38.435	22.961	1.00 30.27
•	ATOM	5911	OH2	TIP	321	37.796	96.408	-12.774	1.00 61.55
	ATOM	5912	OH2	TIP	322	19.428	69.397	2.023	1.00 33.71
20	ATOM	5913	OH2	TIP	323	57.496	90.636	1.067	1.00 54.98
	MOTA	5914	OH2	TIP	324	12.053	82.679	19.654	1.00 38.70
	ATOM	5915	OH2	TIP	325	88.445	13.028	2.038	1.00 43.48
	ATOM	5916	OH2	TIP	326	69.293	34.255	-4.128	1.00 36.68
	ATOM	5917	OH2	TIP	327	. 70.958	38.574	-3.994	1.00 40.96
25	MOTA	5918	OH2	TIP	328	85.340	0 60.784	14.081	1.00 43.08
	MOTA	5919	OH2	TIP	329	15.96	6 91.329	-4.428	
	ATOM	5920	OH2	TIP	330	20.24	5 87.313	3 26.799	
	ATOM	5921	OH2	TIP	331	4.48	9 97.00	7 19.737	•
	ATOM	5922	OH2	TIP	332	85.22	4 40.20	7 1.203	1.00 40.83
30	ATOM	5923	OH2	TIP	333	33.13	4 94.96	2 -3.857	
	ATOM	5924	ОН2	2 TIP	334	81.53	66.87	7 20.22	1 1.00 41.87
	ATOM	5925	OH	2 TIP	335	22.50	5 114.68	6 12.03	
	ATOM	5926	OH	2 TIP	336	51.44	46.90	9 13.06	4 1.00 66.48
	TER	5927	•	TIP	336				
35	ATOM	5928	C1	GOL	529	79.43	36 25.57	10 17.94	8 1.00 44.78

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	ATOM	5929	01	GOL	529		80.194	24.757	17.061	1.00	44.32
	MOTA	5930	C2	GOL	529,		77.910	25.395	17.624	1.00	46.09
	ATOM	5931	02	.GOL	529		77.242	24.886	18,794	1.00	45.98
•	ATOM	5932	С3	GOL	529		77.690	24.402	16.446	1.00	47.19
5	ATOM	5933 ·	03	GOL	° 529		76.335	24.396	15.965	1.00	45.74
	MOTA	5934	C1	GOL	530		78.715	26.772	9.652	1.00	54.03
	MOTA	5935	01	GOL	530		79.769	27.605	10.132	1.00	51.36
	MOTA	5936	C2	GOL	530		79.284	25.356	9.258	1.00	55.43
	ATOM.	5937	02	GOL	530		78.624	24.336	10.032	1.00	55.99
10	ATOM	5938	C3	GOL	530	•	80.810	25.270	9.508	1.00	56.69
	MOTA	5939	03	GÒT	530		81.303	23.931	9.405	1.00	58.79
•	ATOM	5940	C1	GOL	531		79.935	36.623	23.917	1.00	28.32
	ATOM	5941	01	GOL	531		79.999	38.046	24.006	1.00	31.93
	ATOM	5942	C2	GOL	531		78.449	36.144	24.139	1.00	29.57
15	ATOM	5943	02	GOL	531	•	77.997	35.405	22.997	1.00	29.88
	MOTA	5944	С3	GOL	531		77.481	37.343	24.380	1.00	29.38
	ATOM	5945	03	GOL	531		76.119	36.913	24.548	1.00	26.36
	ATOM	5946	_ C1	GOL	532		79.310	52.604	22.101	1.00	21.78
•	ATOM	5947	01	GOL	532 .		79.210	53.188	20.791	1.00	17.99
20	ATOM	5948	C2	GOL	532		78.806	51.109	22.092	1.00	14.64
	MOTA	5949	02	GOL	532		79.917	50.290	22.447	1.00	18.34
	MOTA	5950	C3	GOL	532		78.316	50.657	20.683	1.00	21.57
	MOTA	5951	03	GOL	532		77.640	49.388	20.678	1.00	14.27
	ATOM	5952	C1	GOL	533		12.964	90.743	6.167	1.00	35.75
25	MOTA	5953	01	GOL	533		14.136	90.064	6.618	1.00	40.00
	ATOM	5954	C2	GOL	533	•	13.372	92.168	5.655	1.00	35.48
	ATOM	5955	02	GOL	533		13.004	92.274	4.266	1.00	32.20
	ATOM	5956	С3	GOL	533		14.904	92.393	5.800	1.00	31.71
	ATOM	5957	03	GOL	533		15.276	93.767	5.694	1.00	28.86
30	MOTA	5958	C1	GOL	534		55.733	40.012	9.098	1.00	22.83
	MOTA	5959	01	GOL	534		56.861	39.435	9.738	1.00	24.61
	MOTA	5960	C2	GOL	534		56.230	41.193	8.164	1.00	25.10
	ATOM	5961	02	GOL	534		55.900	40.826	6.823	1.00	20.99
	ATOM	5962	С3	GOL	534		57.766	41.387	8.242	1.00	23.90
35	ATOM	5963	03	GOL	534		58.168	42.742	8.018	1.00	25.49

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The three-dimensional structure of the GSK3- β construct based on the derived crystal structure is schematically illustrated in FIGURE 1. The construct includes N-terminal and C-terminal domains with the active site formed between the two domains. The N-terminal domain includes a β -barrel. The active site region includes the ATP binding site, the magnesium binding/catalytic base site, and substrate binding site.

The three-dimensional structure of the GSK3-β construct's active site (including the catalytic site and substrate binding site) based on the derived crystal structure is schematically illustrated in FIGURE 2. The active site includes Pro136 and Phe67 among other amino acid residues.

Structural information of the apoprotein active site can provide a basis for the rational design of ligands leading to therapeutic compounds effective in the treatment of various disease conditions mediated by GSK3- β activity. Thus, the structural information obtained from the crystallographic data can be used to develop a ligand profile and for the rational design of drugs for mediating GSK3- β activity as described below.

GSK3 Structural Representation. As noted above, in one aspect, the invention provides a method for identifying possible therapeutic compounds in the treatment of various disease conditions mediated by GSK3-β activity. The method involves the use of a three-dimensional structural representation of the GSK construct. The three-dimensional structural representation may be a representation of (a) the complete GSK construct, (b) a fragment of GSK3 that includes the GSK construct, or (c) a fragment of the GSK construct that includes the amino acids that interact with ligands that can mediate GSK3 activity.

The structural representation is preferably based on or derived from the atomic coordinates as set out in Table 2, which represents the structure of the complete GSK construct. Suitable structural representations include three-dimensional models and molecular surfaces derived from these atomic coordinates. The coordinates in Table 2 include structural water and glycerol molecules. These will vary, and may even be absent, in other models derived structurally (they are resolution and space group dependent). These solvent molecules will vary from crystal to crystal.

Variants of the atomic coordinates noted in Table 2 can also be used for the invention, such as variants in which the RMS deviation of the x, y, and z coordinates

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for all heavy (i.e., not hydrogen) atoms are less than about 2.5Å, for example, less than about 2Å, preferably less than about 1Å, more preferably less than about 0.5Å, or most preferably less than about 0.1Å) compared with the atomic coordinates noted in Table 2. Coordinate transformations that retain the three-dimensional spatial relationships of atoms can also be used to give suitable variants.

The atomic coordinates provided herein can also be used as the basis of models of further protein structures. For example, a homology model could be based on the GSK construct structure. The coordinates can also be used in the solution or refinement of further crystal structures of GSK3, such as co-crystal structures with new ligands.

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GSK3 Structural Representation Storage Medium. The atomic coordinates of the GSK construct can be stored on a medium for subsequent use with a computational device, such as a computer (e.g., supercomputer, mainframe, minicomputer, or microprocessor). Typically, the coordinates are stored on a medium useful to hold large amounts of data, such as magnetic or optical media (e.g., floppy disks, hard disks, compact disks, magneto-optical media ("floptical" disks, or magnetic tape) or electronic media (e.g., random-access memory (RAM), or read-only memory (ROM). The storage medium can be local to the computer, or can be remote (e.g., a networked storage medium, including the Internet). The choice of computer, storage medium, networking, and other devices or techniques will be familiar to those of skill in the structural/computational chemistry arts.

The invention also provides a computer-readable medium for a computer, which contains atomic coordinates and/or a three-dimensional structural representation of the GSK construct. The atomic coordinates are preferably those noted in Table 2 or variants thereof. Any suitable computer can be used in the present invention.

GSK3- β Ligand Profile Development. As noted above, the structural information obtained from the crystallographic data can be used to develop a ligand profile useful for the rational design of compounds for mediating GSK3- β activity. A ligand profile can be developed by taking into account the structural information obtained as described above for the apoprotein. The ligand profile can be further developed and refined with the determination of additional structures of protein with bound ligands. The ultimately developed ligand profile identifies possible therapeutic compounds for mediating GSK3- β activity.

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The ligand profile can be primarily based on a shape interaction between the ligand and the protein ligand binding site. The evaluation of the shape interaction can include consideration of the ligand's conformational properties, ranking ligands based on their ability to achieve low energy conformations compatible with the ligand binding site. The shape interaction can also seek to maximize enthalpic interactions between the ligand and the binding site.

The process of developing a ligand profile can vary widely. For example, the profile can be developed by visual inspection of active site structures by experts. Such an inspection can include the consideration of the binding site and ligand structures and compound database searching. The development of the profile can also consider biological data and structure activity relationships (SAR) as well the consideration of known ligand binding interaction with other similar proteins.

In any event, the ligand profile is developed by considering ligand binding interactions including primary and secondary interactions and results in defining the pharmacophore. The term "pharmacophore" refers to a collection of chemical features and three-dimensional constraints that represent specific characteristics responsible for a ligand's activity. The pharmacophore includes surface-accessible features, hydrogen bond donors and acceptors, charged/ionizable groups, and/or hydrophobic patches, among other features.

In addition to the process for ligand profile development noted above, other structure-based drug design techniques can be applied to the structural representation of the GSK3 construct in order to identify compounds that interact with GSK3 to mediate GSK3 activity. A variety of suitable techniques are available to one of ordinary skill in the art.

Software packages for implementing molecular modeling techniques for use in structure-based drug design include SYBYL (available from Tripos Inc., Oxford AMBER (available from http://www/tripos.com); http://www/oxmol.co.uk/); CERIUS² (available from Molecular Simulations Inc., http://www/msn.com/); INSIGHT II (available from Molecular Simulations Inc., http://www/msn.com/); CATALYST (available from Molecular Simulations Inc., http://www/msn.com/); QUANTA (available from Molecular Simulations Inc., Hypercube Inc., HYPERCHEM (available from http://www/msn.com/); http://www/hyper.com/); FIRST DISCOVERY (available from Schrodinger Inc., http://www/schrodinger.com), MOE (available from Chemical Computing Group,

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http://www/chemcomp.com), and CHEMSITE (available from Pyramid Learning, http://www/chemsite.org/), among others.

The modeling software can be used to determine GSK3 binding surfaces and to reveal features such as van der Waals contacts, electrostatic interactions, and/or hydrogen bonding opportunities. These binding surfaces can be used to model docking of ligands with GSK3, to arrive at pharmacophore hypotheses, and to design possible therapeutic compounds *de novo*.

GSK3-B Ligand Virtual Screening

The three-dimensional structure of the apoprotein, and the structure of the protein's active site in particular, allows for the determination of the fit of compounds into the active site. Utilizing a fast docking program, individual compounds from, for example, a compound database, can be evaluated for active site binding. The fit of a particular compound can be evaluated and scored. Setting a score threshold can then provides a family of compounds as a solution to the virtual screen.

At the first level, the virtual screen takes into account the three-dimensional structure of the apoprotein's active site. At the second level, the virtual screen considers the ligand profile and can utilize information obtained from the determination of the structure of protein with bound ligand. A virtual screen is possible even if there is no structural information on a bound ligand.

Information gained from the virtual screen can be considered to further develop the ligand profile. Alternatively, where the results of the virtual screen indicate a promising compound, the compound can be obtained and screened for the relevant biological activity.

<u>Docking</u>. Docking refers to a process in which two or more molecules are aligned based on energy considerations. Docking aligns the three-dimensional structures of two or more molecules to predict the conformation of a complex formed from the molecules (see, e.g., Blaney & Dixon (1993) *Perspectives in Drug Discovery and Design* 1:301). In the practice of the present invention, molecules are docked with the GSK3 construct structure to assess their ability to interact with GSK3.

Docking can be accomplished by either geometric matching of the ligand and its receptor or by minimizing the energy of interaction. Geometric matching algorithms are preferred because of their relative speed.

Suitable docking algorithms include DOCK (Kuntz et al. (1982) J. Mol. Biol. 161:269-288, available from UCSF), the prototypical program for structure-based

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drug design; AUTODOCK (Goodsell & Olson (1990) Proteins: Structure, Function from Oxford available Molecular, 8:195-202 and Genetics and http://www/oxmol.co.uk/), which docks ligands in a flexible manner to receptors using grid-based Monte Carlo simulated annealing. The flexible nature of the AUTODOCK procedure helps to avoid bias (e.g., in orientation and conformation of the ligand in the active site) introduced by the user searcher (Meyer et al. (1995) Persp. Drug Disc. 3:168-95) because, while the starting conformation in a rigid docking is normally biased towards a minimum energy conformation of the ligand, the binding conformation may be of relatively high conformational energy (Nicklaus et al. (1995) Bioorganic & Medicinal Chemistry 3:411).

Other suitable docking algorithms include MOE-DOCK (available from Chemical Computing Group Inc., http://www/chemcomp.com), in which a simulated annealing search algorithm is used to flexibly dock ligands and a grid-based energy evaluation is used to score docked conformations; FLExX (available from Tripos Inc., http://www/tripos.com), which docks conformationally flexible ligands into a binding site using an incremental construction algorithm that builds the ligand in the site, and scores docked conformations based on the strength of ligand-receptor interactions; GOLD (Jones et al. (1997) J. Mol. Biol. 267:727-748), a genetic algorithm for flexible ligand docking, with full ligand and partial protein flexibility, and in which energy functions are partly based on conformation and non-bonded contact information; AFFINITY (available from Molecular Simulations Inc., http://www/msn.com/), which uses a two step process to dock ligands: first, initial placements of the ligand within the receptor are made using a Monte Carlo-type procedure to search both conformational and Cartesian space; and second, a simulated annealing phase optimizes the location of each ligand placement, during this phase, AFFINITY holds the "bulk" of the receptor (atoms not in the binding site) rigid, while the binding site atoms and ligand atoms are movable; C2 LigandFit (available from Molecular Simulations Inc., http://www/msn.com/), which uses the energy of the ligand-receptor complex to automatically find best binding modes and stochastic conformation search techniques, with the best results from the conformational sampling retained. A grid method is used to evaluate non-bonded interactions between the rigid receptor and the flexible ligand atoms. DOCKIT (available from Metaphorics LLC) uses distance geometry for fast flexible ligand docking. GLIDE (available from Schrodinger Inc.) uses a pre-computed energy grid and an efficiently pruned systematic search for flexible docking.

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Preferably, the docking algorithm is used in a high-throughput mode, in which members of large structural libraries of potential ligands are screened against the receptor structure (Martin (1992) *J. Med. Chem.* 35:2145-54).

Suitable structural libraries include the ACD (Available Chemical Directory, form MDL Inc.), AsInEx, Bionet, ComGenex, the Derwent World Drug Index (WDI), the Contact Service Company database, LaboTest, ChemBridge Express Pick, ChemStar, BioByteMasterFile, Orion, SALOR, TRIAD, ILIAD, the National Cancer Institute database (NCl), and the Aldrich, Fluka, Sigman and Mabridge catalogs. These are commercially available (e.g., the *HTS Chemicals* collection from Oxford Molecular, or the LeadQuestTM files from Tripos).

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<u>Defining the Pharmacophore</u>. As noted above, a pharmacophore can be defined for the GSK3 construct that includes surface-accessible features, hydrogen bond donors and acceptors, charged/ionizable groups, and/or hydrophobic patches, among other features. These features can be weighted depending on their relative importance in conferring activity (see, e.g., *Computer-Assisted Lead Finding and Optimization* (eds. Testra & Folkers, 1997).

Pharmacophores can be determined using software such as CATALYST (including HypoGen or HipHop, available from Molecular Simulations Inc., http://www/msn.com/), CERIUS², or constructed by hand from a known conformation of a lead compound. The pharmacophore can be used to screen structural libraries, using a program such as CATALYST. The CLIX program (Davic & Lawrence (1992) *Proteins* 12:31-41) can also be used, which searches for orientations of candidate molecules in structural databases that yield maximum spatial coincidence with chemical groups which interact with the receptor. The DISCO program (available from Tripos) uses a method of clique detection to identify common pharmacophoric features in each structure, produce optimally aligned structures, and extract the key features of the pharmacophore. The GASP program (available from Tripos) uses a genetic algorithm to automatically find pharmacophores with conformational flexibility.

<u>de novo Compound Design</u>. The binding surface or pharmacophore of the GSK3 construct can be used to map favorable interaction positions for functional groups (e.g., protons, hydroxyl groups, amine groups, acidic groups, hydrophobic groups and/or divalent cations) or small molecule fragments. Compounds can then be designed *de novo* in which the relevant functional groups are located in the correct spatial relationship to interact with GSK3.

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Once functional groups or small molecule fragments which can interact with specific sites in the binding surface of GSK3 have been identified, they can be linked in a single compound using either bridging fragments with the correct size and geometry or frameworks which can support the functional groups at favorable orientations, thereby providing a compound according to the invention. While linking of functional groups in this way can be done manually, perhaps with the help of software such as QUANTA or SYBYL, automated or semi-automated *de novo* design approaches can also be used.

Suitable de novo design software includes MCDLNG (Gehlhaar et al. (1995) J. Med. Chem. 38:466-72), which fills a receptor binding site with a close-packed array of generic atoms and uses a Monte Carlo procedure to randomly vary atom types, positions, bonding arrangements and other properties; MCSS/HOOK (Caflish et al. (1993) J. Med. Chem. 36:2142-67; Eisen et al. (1994) Proteins: Str. Funct. Simulations Inc., Molecular from 19:199-221; available Genet. http://www/msn.com), which links multiple functional groups with molecular templates taken from a database; LUDI (Bohm (1992) J. Comp. Aided Molec. Design 6:61-78, available from Molecular Simulations Inc., http://www/msn.com), which computes the points of interaction that would ideally be fulfilled by a ligand, places fragments in the binding site based on their ability to interact with the receptor, and then connects them to produce a ligand; GROW (Moon and Howe (1991) Proteins: Str. Funct. Genet. 11:314-328), which starts with an initial "seed" fragment (placed manually or automatically) and grows the ligand outwards; SPROUT (available from http://chem.leeds.ac.uk/ICAMS/SPROUT.html), which includes molecules to identify favorable hydrogen bonding and hydrophobic regions within a binding pocket (HIPPO module), selects functional groups and positions them at target sites to form starting fragments for structure generation (EleFanT), generates skeletons that satisfy the steric constraints of the binding pocket by growing spacer fragments onto the start fragments and then connecting the resulting part skeletons (SPIDeR), substitutes hetero atoms into the skeletons to generate molecules with the electrostatic properties that are complementary to those of the receptor site (MARABOU), and the solutions can be clustered and scored using the ALLigaTOR module; LEAPFROG (available from Tripos Inc., http://www/tripos.com), which evaluates ligands by making small stepwise structural changes and rapidly evaluating the binding energy of the new compound, keeps or discards changes based on the altered binding energy, and evolves structures to increase the interaction energy with WO 02/24893 PCT/US01/29549

the receptor; GROUPBUILD (Rorstein et al. (1993) J. Med. Chem. 36:1700), which uses a library of common organic templates and a complete empirical force field description of the non-bonding interactions between a ligand and receptor to construct ligands that have chemically reasonable structure and have steric and electrostatic properties complimentary to the receptor binding site; CAVEAT (Lauri and Bartlett (1994) Comp. Aided Mol. Design 8:51-66), which designs linking units to constrain acyclic molecules; and RASSE (Lai (1996) J. Chem. Inf. Comput. Sci. 36:1187-1194).

GSK3-β Ligands

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Most lead compounds that initiate structure-based design cycles are identified by high-throughput screening. As a result of high throughput screening and the ligand profile and virtual screening described above, ligands are identified having the requisite conformational energies to assume a suitable shape and bind with the protein's active site. In addition to having low conformational energy and spatial compatibility with the apoprotein active site, the identified ligands are preferably synthetically accessible. The identified ligands can then be obtained (e.g., commercially obtained or synthesized) and screened for biological activity. The identified ligands can also be co-crystallized with the protein construct and the three-dimensional structure determined for the protein with bound ligand. The information obtained from structure of the protein with bound ligand can then be used to further develop the ligand profile as described above.

Suitable GSK3- β biological screening methods for evaluating ligand biological activity are known and include, for example, those noted in U.S. patent application Serial No. 60/193,043, filed March 29, 2000, and expressly incorporated herein be reference in its entirety.

Method for Rational Drug Discovery Using GSK3 Crystal Structures

In another aspect, the invention provides a method for using a GSK3 crystal structure, specifically the three-dimensional structure of the GSK3 construct's active site, to design ligands for binding to and mediating the activity of GSK3-β.

In one embodiment, the method is an iterative structure-based method for therapeutic compound design. A representative method is depicted by the flow diagram shown in FIGURE 3. Referring to FIGURE 3, the crystal structures of the apoprotein and the protein with bound ligand are determined in steps 102 and 104, respectively. From the structural information obtained from steps 102 and 104, a ligand profile is developed in step 106. A ligand profile can also be developed

directly from the crystal structure of the apoprotein. Using the resulting profile, new ligands can be designed and/or obtained, screened for biological activity, and/or co-crystallized with the protein in step 108, or alternatively, the ligand profile can be used in a virtual screen in step 110. If the ligand obtained from the developed profile is co-crystallized, the structure of the co-crystal is determined in step 104 and the resulting structural information is used to further develop the ligand profile in step 106. If the ligand profile is used in a virtual screen in step 110, the virtual screen is either successful and identifies one or more ligands that can be obtained, screened, and/or co-crystallized in step 108. If the virtual screen is unsuccessful in identifying a suitable ligand, the ligand profile is further developed in step 106.

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Lead compounds can be identified from biological screening of ligands developed by the ligand profile. A representative method for identifying a lead compound is depicted by the flow diagram shown FIGURE 4. Referring to FIGURE 4, the crystal structures of the apoprotein and the protein with bound ligand are determined in steps 202 and 204, respectively. From the structural information obtained from steps 202 and 204, a ligand profile is developed in step 206. A ligand profile can also be developed directly from the crystal structure of the apoprotein. From the resulting profile, a new ligand can be designed and/or obtained in step 208, and either screened for biological activity in step 210 and/or co-crystallized with the protein in step 212. If the biological screen is successful, a lead compound is identified in step 214. In a subsequent iteration, the lead compound can be cocrystallized in step 212 and iterations continued until a new drug candidate is identified. If the biological screen is not successful, that information can be used to further develop the ligand profile in step 206. If the ligand is co-crystallized, the cocrystal structure can be determined in step 204 and the structural information used in further developing the ligand profile in step 206.

Alternatively, the results of the ligand profile can be used in a virtual screen in step 216. If the virtual screen is successful and identifies one or more ligands, the ligand can be obtained in step 208 and screened in step 210 to determine its biological activity and whether or not a lead compound has been identified. The ligand obtained in step 208 can also be co-crystallized in step 212 and its structure determined and the resulting information used to further develop the ligand profile. If the virtual screen is unsuccessful in identifying a suitable ligand, the ligand profile is further developed in step 206.

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GSK3 Ligands and Their Uses

The method of the invention identifies ligands that can interact with GSK3. These compounds can be designed *de novo*, can be known compounds, or can be based on known compounds. The compounds can be useful pharmaceuticals themselves, or can be prototypes that can be used for further pharmaceutical refinement (i.e., lead compounds) in order to improve binding affinity or other pharmacologically important features (e.g., bio-availability, toxicology, metabolism, pharmacokinetics).

Accordingly, in another aspect, the invention provides (1) a compound identified using the method of the invention; (2) a compound identified using the method of the invention for use as a pharmaceutical; (3) the use of a compound identified using the method of the invention in the manufacture of a medicament for mediating GSK3 activity; and (4) a method of treating a patient afflicted with a condition mediated by GSK3 activity that includes administering an amount of a compound identified using the method of the invention that is effective to mediate GSK3 activity.

These compounds preferably interact with GSK3 with a binding constraint in the micromolar or, more preferably, nanomolar range or stronger.

As well as being useful compounds individually, ligands identified by the structure-based design techniques can also be used to suggest libraries of compounds for traditional *in vitro* or *in vivo* screening methods. Important pharmaceutical motifs in the ligands can be identified and mimicked in compound libraries (e.g., combinatorial libraries) for screening for GSK3-binding activity.

The foregoing and other aspects of the invention may be better understood in connection with the following representative examples.

EXAMPLES

Example 1

GSK3-β Construct Purification

In this example, the purification of the GSK3- β protein construct is described. The construct was extracted from SF-9 cells infected with a baculovirus carrying GSK3- β 580 cDNA construct and purified to apparent homogeneity using S-Fractogel, Phenyl-650 M, and Glu-tag affinity chromatographies as described below.

Extraction. Cell paste from 20L fermentation of infected SF-9 cells was washed 100 mL PBS (10 mM NaPi, pH 7.5, 150 mM NaCl) and then resuspended

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with 300 mL of Buffer H (20 mM Tris, pH 7.5, 1 mM tungstate, 1 mM arsenate, 50 mM DTT, 10 μ g/mL leupeptin, 1 μ g/mL pepstatin A, 10% glycerol, 0.35% octyl glycoside, 1 mM Mg²⁺). Cells were homogenized in a 100-mL Douncer (20 strokes with pestel B). The combined homogenate was centrifuged in a Ti45 rotor at 40,000 rpm for 35 minutes to remove cell debris and nuclei. The supernatant from the centrifugation were carefully decanted and filtered through 0.45 μ filter.

S-Fractogel Chromatography. 175 mL S-fractogel (EM Science, Cat #18882) was packed into 5 cm x 8.9 cm column and equilibrated with 5 column volumes of Buffer A (20 mM Tris, Ph 7.5, 10% glycerol). Prior to loading the filtered supernatant, one column volume of Buffer A containing 50 mM DTT was passed over the equilibrated column. The filtrate from the previous step was then loaded at 20 mL/min onto the column. The column was washed with 3 column volumes of Buffer A containing 50 mM DTT and 2 column volumes of Buffer A and then eluted with a linear gradient from 0 to 1 M NaCl in Buffer A over 20 column volumes. The eluant was fractionated into 20 mL fractions. Fractions containing GSK3 were detected by Western Blot using anti-GSK antibody (Santa Cruz Biotech, Cat # SC-7291). The Western-Blot positive fractions were pooled and mixed with equal volume of Buffer M (20 mM Tris, pH 7.5, 10% glycerol, 3.1 M NaCl) and filtered through a 0.45 μ filter. The filtrate was used for Phenyl-650 M chromatography.

Phenyl-650 M Chromatography. 37.5 mL Phenyl-650 M (Tosohass, Cat #014943) was packed into a 2.2 x 10 cm column and equilibrated with 5 column volumes of Buffer C (20 mM Tris, pH 7.5, 10% glycerol, 1.6 M NaCl). Filtrate from S-fractogel step was loaded onto the column at 7.5 mL/min. After the loading was completed, the column was washed with 5 column volumes of Buffer C and eluted with linear gradient from 0% to 100% Buffer A (20 mM Tris, pH 7.5, 10% glycerol) over 20 column volumes. Fractions were collected at 15 mL each and GSK containing fractions were detected by Western Blot using anti-GSK antibody. The Western positive fractions were pooled and loaded onto a Glu-tag antibody affinity column.

Glu-tag Affinity Chromatography. 50 mg of Glu-tag antibody was immobilized onto 28 mL of Affi-Gel 10 (BioRAD, Cat #153-6046) and the packed into 2.2 x 6.5 cm column. The column was equilibrated with 5 column volumes of Buffer D (20 mM Tris, pH 7.5, 20% glycerol, 0.3 M NaCl, 0.2% octylglucoside) and the fraction pool from Phenyl-650 M step was loaded at 2.8 mL/min. After the

loaded was completed, the column was wash with 5 column volumes of Buffer D and then eluted with 100 mL Glu-tag peptide (100 µg/mL) in Buffer D and fractionated into 4 mL fractions. GSK containing fractions were detected with SDS-PAGE and Coomassie Blue staining. These fractions were pooled, concentrated, and diafiltered into Buffer D to approximately 4.8 mg/mL in an Amicon concentrator using a 10 k MWCO YM10 membrane. The concentrated material was then submitted for crystallization.

Example 2

GSK3-B Construct Crystallization

In this example, the crystallization of the GSK3-β protein construct is described. Crystallization protocol utilizes GSK3β at a concentration of 4.8 mg/ml and in a solution containing 1X TBS buffer, 0.3 M NaCl, 20% glycerol, 0.2 % octyl glucopyranoside, 5 mM DTT,. The crystals were grown by the vapor diffusion using the hanging drop method. Briefly, each well of a 24-well linbro culture plate was filled with 0.5 mL of a solution containing 10% polyethylene glycol 6000 (PEG 6000), 5% 2-methyl-2,4-pentanediol (MPD), 0.1 M HEPES, pH 7.5. 3 uL of protein solution was then mixed with 3 uL of well solution in a drop on a glass cover slip. The cover slip was then placed over the reservoir of the well. The plate was then stored at 4°C. Crystals appeared in 50-90% of the wells in 3-30 days.

Representative GSK3 crystals are highly polymorphic and exhibit variance in both the space-group and unit cell dimensions, often showing space group transitions during compounds soaking and in response to subtle changes in conditions. Three space groups have been identified in GSK3 crystals and are given below. The space group dimensions in all the space groups and the beta angle in space group C2 can often vary by as much as 10% between individual crystals. The space group and dimensions are as follows. C222(1) is the most prevalent space group, followed by C2, and then P222(1). C2 is seen only when a compound has been soaked into the crystal.

C222(1): a=89.874 b=102.514 c=108.194 alpha=90 beta=90 gamma=90

C2: a=102.366 b=89.598 c=110.438 alpha=90 beta=96.983 gamma=90

P222(1): a=86.328 b=103.061 c=102.846 alpha=90 beta=90 gamma=90

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The crystals can be cryoprotected for data collection in a cryosolution consisting of 12% PEG 6000, 11% MPD, 0.1 M HEPES pH 7.5, 20% glycerol. The the cryosolution can include from about 10 to about 14 percent by weight polyethylene glycol (PEG 6000), from about 9 to about 13 percent by weight 2-methyl-2,4-pentanediol (MPD), and from about 18 to about 22 percent by weight glycerol. The cryosolution can have a pH of from about 7.3 to about 7.7.

Example 3

GSK3-β Construct Crystal Structure Resolution

In this example, a representative method for resolving the crystal structure of the GSK3- β protein construct is described.

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The crystal structure of GSK3 β was solved using a combination of molecular replacement and cross-crystal averaging. A molecular replacement solution for the C222(1) crystal form was obtained using a homology model of GSK3β (containing residues 53-352) and the program EPMR [CR Kissinger, DK Gehlhaar, and DB Fogel. Rapid automated molecular replacement by evolutionary search. Acta Crystallogr D Biol Crystallogr. 1999 Feb;55 (Pt 2):484-91]. The homology model was constructed using the phosphorylated form of CDK2 (PDB accession code 1JST) as the template. This initial molecular replacement solution gave a model with an R-factor of 53.9%. The model was then processed through several rounds of a A typical refinement macrocycle consists of 100-200 refinement macrocycle. rounds of conjugate gradient minimization, simulated annealing with either torsion or Cartesian dynamics, and grouped or individual temperature factor calculation. All refinement procedures were executed using the program CNX (Molecular Simulation, Inc.) This was followed by calculation of new electron density maps and manual rebuilding of the model based on features within these maps using the program O (DATAONO AB). All data from 30Å-2.8Å in the C222(1) set of data was used. Despite numerous macrocycles of refinement, it was not possible to improve the model to better than an R-factor of 35% (free-R factor of 0.41). This bias towards an incorrect structure was caused by the lack of high-resolution data and the low ratio of parameters to measurable data in the refinement.

To alleviate this bias, cross-crystal averaging was used to improve the phases provided by the initial molecular replacement solution. In cross-crystal averaging, two or more separate "views" of a structure are obtained from crystals of vastly different unit cell dimensions and/or space-groups. The electron densities of these views are then averaged together to provide more accurate phases for the Fourier

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reconstruction of the electron density and an improved view of the actual electron density within each of the separate crystals. For the cross-crystal averaging, the C222(1) crystal data set and C2 crystal data set (obtained from soaking a GSK3ß crystal in 1-3 mM of Compound 1 (illustrated below) were used. Two molecular replacement solutions were obtained for the C2 crystal form using the partially refined GSK3\beta model; these solutions represented the two molecules of GSK3\beta in the asymmetric unit of the C2 cell. The real-space transforms between the molecule in the C222(1) crystal form and the molecules in the C2 crystal form were then calculated. Following this, the phases and figures-of-merit from an ensemble of 10 structures run through the refinement macrocycle in the C222(1) crystal form were averaged against the data from the C2 crystal form using the program DMMULTI [K. Cowtan. Joint CCP4 and ESF-EACBM Newsletter on Protein Crystallography 1994; 31, pp 34-38] and all data to 2.7 Å. One hundred cycles of averaging, solventflattening, and histogram matching were performed. Following this, improved electron density maps were calculated and the model was rebuilt, followed by another refinement macrocycle, and another round of cross-crystal averaging. Five total averaging/refinement cycles were performed. In cycles 2-5, major errors were found in the C222(1) model and corrected, and the rest of the macromolecule was built (residues 37-384). The final C222(1) crystal structure consists of the biologically relevant molecule, 79 waters, and one putative chloride ion, and has an R-factor of 22.46% and a free-R factor of 28.22% using data from 30Å-2.7Å.

Compound 1:

Following the completion of the refinement of C222(1) crystal structure, the resulting model and molecular replacement were then used to determine the position and structure of the molecule in the two soaked-compound C2 crystals and the P222(1) crystal. The current best GSK3β structure is from a P222(1) crystal form

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obtained during a soak with Compound 2 (illustrated below) which diffracts to 2.2Å. This structure consists of two copies of the biologically relevant macromolecule in the asymmetric unit, 336 waters, 6 glycerols; this structure has an R-factor of 26.2% and free-R factor of 30.8% using data from 30 Å-2.2 Å. Compound 2 has not reached high enough occupancy in the active site to be observed.

Compound 2:

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This approach was used to determine the structure due to the limiting nature of available data collection facilities at the time. More traditional methods such as single/multiple isomorphous replacement or MAD phasing by themselves or in conjunction with molecular replacement could have been used equally as well. A description of these methods and other crystallographic principles can be found in B.K. Shoichet and D.E. Bussiere, The role of macromolecular crystallography and structure for drug discovery: advances and caveats. Current Opinion in Drug Discovery & Development 2000; 3(4): 408-422.

While the preferred embodiment of the invention has been illustrated and described, it will be appreciated that various changes can be made therein without departing from the spirit and scope of the invention.

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The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

- 1. A method for providing an atomic model of a GSK3 protein, comprising:
- (a) providing a computer readable medium having stored thereon atomic coordinate/x-ray diffraction data of the GSK3 protein in crystalline form, the data sufficient to model the three-dimensional structure of the GSK3 protein;
- (b) analyzing the atomic coordinate/x-ray diffraction data from (a) to provide data output defining an atomic model of the GSK3 protein; and
- (c) obtaining atomic model output data defining the three-dimensional structure of the GSK3 protein.
- 2. A computer readable medium having stored thereon atomic model data of the GSK3 protein produced by the method of Claim 1.
- 3. A GSK3-β ligand corresponding to the physical model of the atomic model of the ligand model produced by the method of Claim 1.
- 4. A method for designing ligands that bind to a GSK3 protein, comprising using some or all of the atomic coordinates of the GSK3 construct presented in Table 2.
- 5. A method for designing ligands that bind to a GSK3 protein, comprising:
 - (a) providing a purified GSK3 protein;
- (b) crystallizing the purified GSK3 protein to provide a crystallized GSK3 protein having biological activity;
- (c) resolving the structure of the crystallized GSK3 protein using x-ray crystallography to obtain data suitable for three-dimensional structure determination of the GSK3 protein;
- (d) applying the data generated from resolving the structure of the crystallized GSK3 protein to a computer algorithm to generate a model of the GSK3 protein suitable for use in designing ligands that will bind to the GSK3 protein active site; and
- (e) applying an iterative process whereby molecular structures are applied to the computer generated model to identify GSK3 binding ligands.

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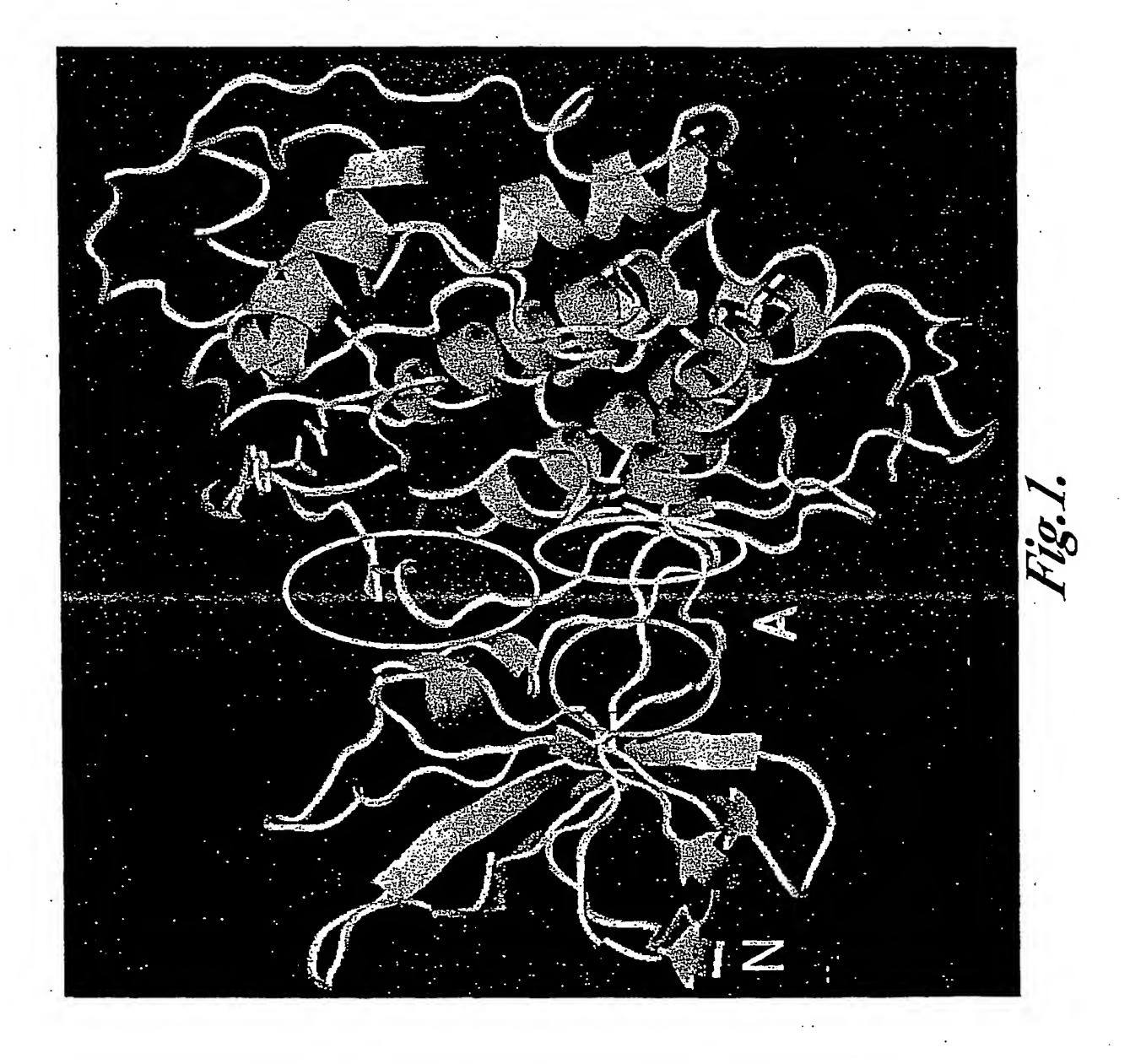
- 6. The method of Claim 5, wherein the protein comprises the atomic coordinates set forth in Table 2.
- 7. The method of Claim 5, wherein the protein comprises the amino acid sequence set forth in SEQ ID NO: 1 or an active mutant or variant thereof.
- 8. A GSK binding ligand designed by the method of any one of Claims 4-7.
- 9. A method for identifying a GSK3 mediator by determining the binding interactions between a potential mediator and a GSK3 binding site, the binding site being defined by at least some of the atomic coordinates set forth in Table 2, the method comprising:
- (a) generating a binding cavity defined by the binding site on a computer screen;
 - (b) generating compounds with their spatial structure; and
 - (c) determining whether the compounds bind at the GSK3 binding site.
- 10. A method for identifying a compound that mediates GSK3 activity, comprising:
- (a) designing a potential mediator for GSK3 that will form non-covalent bonds with amino acids in the GSK3 binding site based on at least some of the atomic structure coordinates set forth in Table 2;
 - (b) obtaining the potential mediator; and
- (c) determining whether the potential mediator mediates the activity of GSK3.
- 11. A method for identifying a compound that mediates GSK3 activity, comprising:
- (a) using a three-dimensional structure of GSK3 as defined by the atomic coordinates set forth in Table 2 to design or select the potential mediator;
 - (b) obtaining the potential mediator; and
- (c) contacting the potential mediator with GSK3 to determine whether the potential mediator mediates the activity of GSK3.
- 12. A computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex

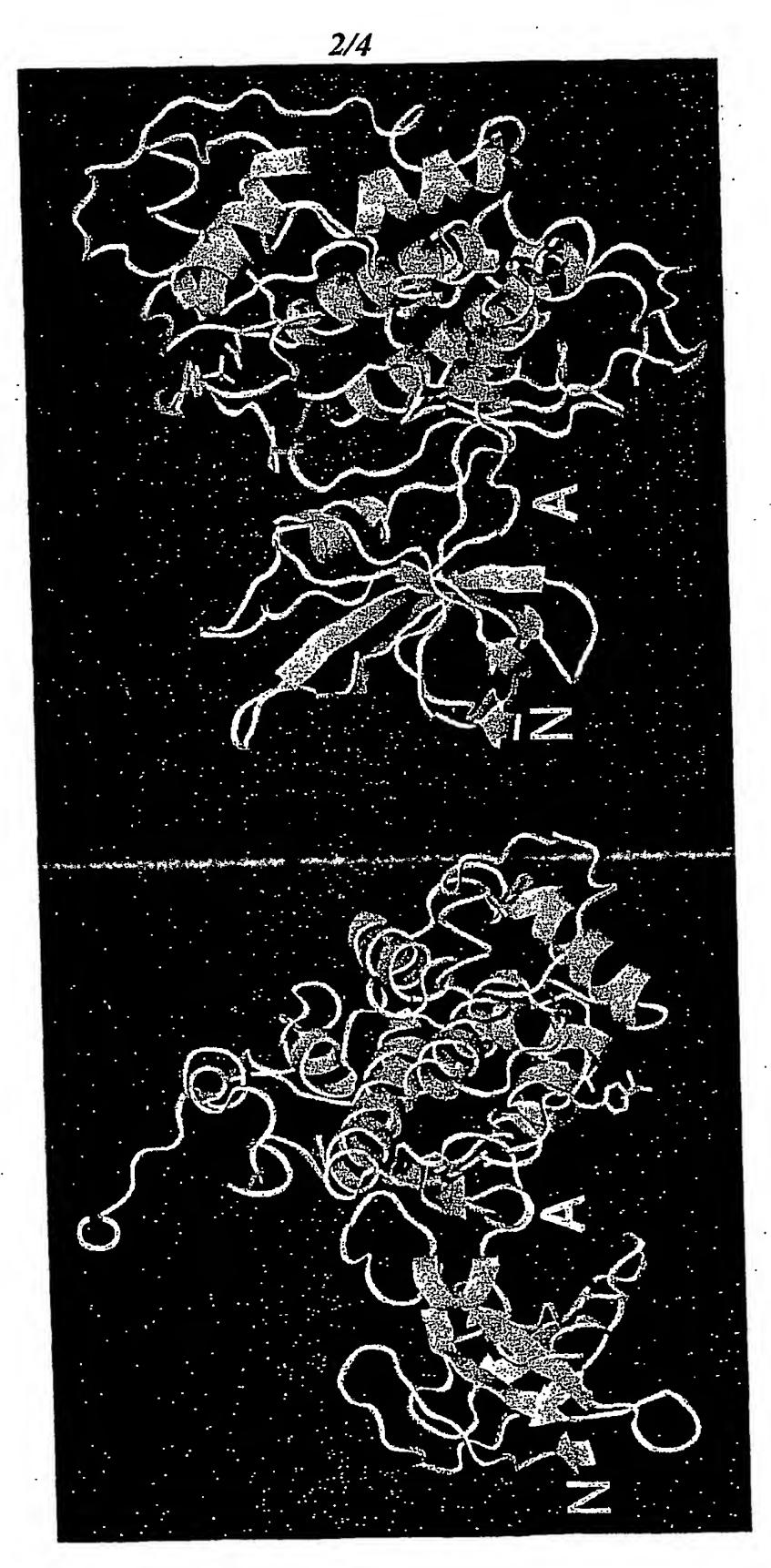
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comprises a binding pocket defined by at least some of the atomic coordinates of GSK3 provided in Table 2, or a three-dimensional representation of a homologue of the molecule or molecular complex, wherein the computer comprises:

- (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the atomic coordinates set forth in Table 2;
- (b) a working memory for storing instructions for processing said machine-readable data;
- (c) a central-processing unit coupled to said working memory and to said machine-readable data storage medium for processing said machine readable data into said three-dimensional representation; and
- (d) a display coupled to said central-processing unit for displaying said three-dimensional representation.
- 13. A computer for determining at least a portion of the atomic coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex, wherein said computer comprises:
- (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the atomic coordinates set forth in Table 2;
- (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
- (d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and
- (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.
- 14. A method for crystallizing a human glycogen synthase kinase 3 (GSK3) protein, comprising:
 - (a) providing a purified GSK3 protein; and

- (b) crystallizing the purified GSK3 protein to provide a crystallized GSK3 protein having biological activity, wherein the protein is crystallized from a solution comprising from about 10 to about 14 percent by weight polyethylene glycol, from about 9 to about 13 percent by weight 2-methyl-2,4-pentanediol, and from about 18 to about 22 percent by weight glycerol, and wherein the crystallized GSK3 protein is resolvable using x-ray crystallography to obtain x-ray patterns suitable for three-dimensional structure determination of the GSK3 protein.
- 15. The method of Claim 14, wherein crystallizing the GSK3 protein comprises crystallizing by a hanging drop vapor diffusion method.
- 16. The method of Claim 14, wherein the protein comprises the atomic coordinates set forth in Table 2.
- 17. The method of Claim 14, wherein the protein comprises the amino acid sequence set forth in SEQ ID NO: 1 or an active mutant or variant thereof.
 - 18. A crystallized GSK3 protein provided by the method of Claim 14.





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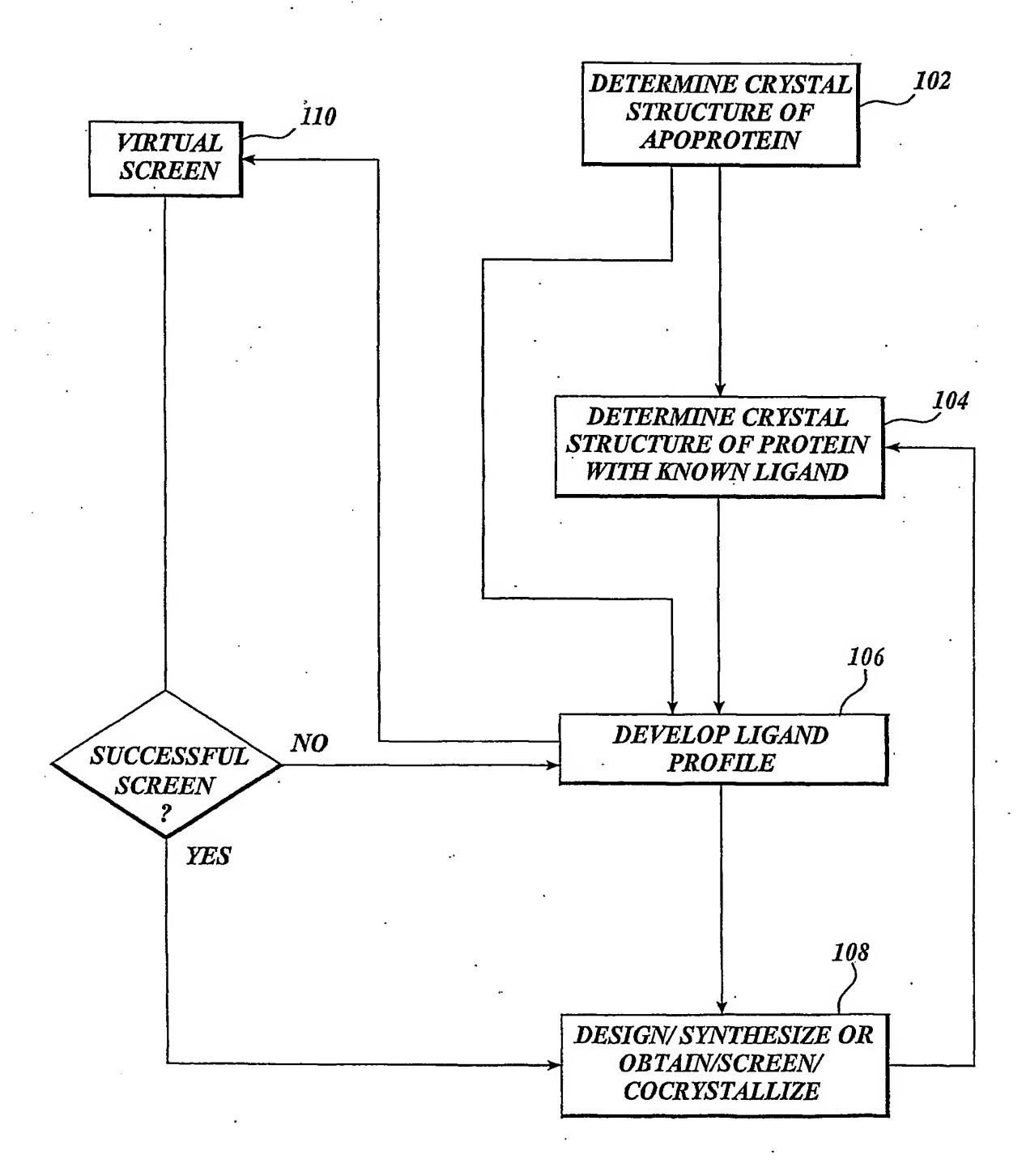


Fig. 3

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